UNIVERSITY OF OXFORD

Doctor of Philosophy

The role of green ammonia in decarbonised energy systems

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Submitted May 2022

Submitted with Revisions November 2022

Abstract

Green ammonia is gaining momentum as a globally significant technology for deep decarbonisation. In this thesis, several models are developed across chemical, techno-economic, and energy system modelling disciplines to explore the future role of green ammonia. First, standalone models of production (i.e., power-to-ammonia) and re-electrification (i.e., ammonia-to-power) are developed and compared to competing technologies. Second, these models are integrated into a planning and dispatch energy system model (ESM) of India to 2050. The ESM has several novel additions including the sector coupling of hydrogen and ammonia, multiple years of granular weather data, and learning-curve-based technology cost forecasts. India is chosen as an ideal case study given its globally unmatched demand growth in all three relevant sectors: electricity, green hydrogen, and green ammonia. The projected electricity demands for green hydrogen and ammonia production account for 25% of the total Indian electricity demand in 2050, underscoring the transformational potential that green hydrogen and ammonia sector coupling can have on the Indian energy system.

The results of the state-of-the-art ESM highlight synergistic effects of hydrogen and ammonia sector coupling with the power system. The least-cost system employs seasonal green ammonia production paired with up to 40 million tonnes (i.e., 200 TWh) of ammonia storage, as well as some re-electrification via gas turbines. Sector coupling reduces system curtailment, addresses challenges of long-duration storage, and improves system resilience to interannual weather variations. While India is a crucial case study from a global decarbonisation perspective, the methodology and findings are generally applicable, and it is the aim of this work to motivate and accelerate the wider research community into considering the potential impacts of green ammonia sector coupling on electricity grid design. Finally, this work highlights strategic technology development direction for ammonia producers and gas turbine manufacturers, as well as implications for policymakers.

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

Publications and Presentations

Journal Papers

Submitted **Cesaro, Z.**, Bramstoft, R., Ives, M., & Bañares-Alcántara, R. *Facilitating deep decarbonization via sector coupling of green hydrogen and ammonia.* (2022)

- **Cesaro, Z.**, Ives, M., Nayak-Luke, R., Mason, M. & Bañares-Alcántara, R. *Ammonia to power: Forecasting the levelized cost of electricity from green ammonia in large-scale power plants.* Applied Energy **282**, 116009. (2021)

Book Chapters

- **Z. Cesaro**, R. M. Nayak-Luke and R. Bañares-Alcántara, "Chapter 2 - Energy Storage Technologies: Power-to-X," in Techno-Economic Challenges of Green Ammonia as an Energy Vector, Academic Press, 2020, pp. 15-26.
- R.M. Nayak-Luke, **Z. Cesaro**, R. Bañares-Alcántara, "Chapter 3 - Pathways for Green Ammonia," in Techno-Economic Challenges of Green Ammonia as an Energy Vector, Academic Press, 2020, pp. 27-39.
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Selected Presentations

- Z. Cesaro, "The role of green ammonia in sector coupling and seasonal electricity storage," Ammonia Energy Association Conference 2021, Boston, AEA, Nov 2021.
- Z. Cesaro, "Exploring Hydrogen via Risk- Opportunity Analysis (ROA) in India," Risk-Opportunity Approach to Technology Dynamics: Third Workshop of the EEIST Research Consortium: India Community of Practice, Delhi (virtual), EEIST, Sep 2021.
- Z. Cesaro, "The Fuel of the Future: Behind the Scenes with Green Ammonia," TEDx Oxford, Feb 2021. https://www.ted.com/talks/zac_cesaro_the_fuel_of_the_future_behind_the_scenes_with _green_ammonia.
- Z. Cesaro, "Green ammonia as an energy vector," India's Green Ammonia Opportunity Workshop, Delhi (virtual), OXGATE and CEEW, Nov 2020.

- Z. Cesaro, "Power-to-X: a closer look at e-Ammonia," SRBE-KBVE Webinar: Power to Molecules, The Royal Belgian Society for Electricians, Dec 2020.
- Z. Cesaro, "From demonstration to global green ammonia economy," Tees Valley Hydrogen Webinar, Teeside University, Oct 2020.
- Z. Cesaro, "Siemens Green Ammonia Demonstrator & Investigation into Ammonia for Energy Infrastructure in Developing Countries," UK Energy Storage Conference, Newcastle, Sep 2019.
- Z. Cesaro, "Siemens Demonstrator Update & Investigation into Ammonia for Energy Infrastructure in Developing Countries," NH3 Event, Rotterdam, Jun 2019.

Acknowledgements

First and foremost I would like to thank my primary supervisor Dr. René Bañares-Alcántara for his continued support and guidance throughout this DPhil. It has been an exciting ride for both of us as green ammonia has gained momentum, and I am grateful for his steering towards valuable research questions. I am also deeply thankful to my co-supervisor Dr. Matthew Ives for his insightful energy modelling guidance, encouragement to be bold, and connection to a larger project in the latter half of this DPhil. Additionally, I would like to thank Dr. Ramsus Bramstoft for his patient energy system modelling support and for his keen interest in this project through to the end. Finally, I would like to thank Dr. Ian Wilkinson at Siemens Energy for the opportunities he has consistently given me to apply my research to the real world and for always encouraging me to prioritise the DPhil research.

This research would not have been possible without financial support from various sources. I would like to acknowledge the financial support of the Yeotown Scholarship from New College, and the UK BEIS International Climate Finance, the Children's Investment Fund Foundation (CIFF), and the Oxford Martin School Post-Carbon Transitions (PCT) Programme for supporting this research as part of the Economics of Energy Innovation and System Transition (EEIST) programme (grant number LDR00530). The use of Aspen Plus and MATLAB were used under an AspenTech and MATLAB academic licences respectively.

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Nomenclature

AFC Alkaline Fuel Cell

Balmorel BALtic Model Of Regional Energy Liberalization (historical acronym, no longer relevant)

bcm billion cubic meters

BECCS Bio-energy with Carbon Capture and Storage

BEIS Department for Business, Energy, and Industrial Strategy

BEV Battery Electric Vehicle

BNEF Bloomberg New Energy Finance

CAN Calcium Ammonium Nitrate

CAPEX Capital Expenditure

CBA Cost Benefit Analysis

CCGT Combined Cycle Gas Turbine

CCS Carbon Capture and Storage

CDR Carbon Dioxide Removal

CEA Central Electricity Authority

CF Capacity Factor

CIFF Childern's Investment Fund Foundation

CNG Compressed Natural Gas

DHI Diffuse Horizontal Irradiance

DNI Direct Normal Irradiance

DRI Direct Reduction of Iron ore

EAF Electric Arc Furnace

ECMWF European Centre for Medium-Range Weather Forecasts

EEIST Economics of Energy Innovation and System Transition

ER Eastern Region

ERA5 ECMWF Reanalysis v5

ERI Energy Research Institute

ESM Energy System Model

FCEV Fuel Cell Electric Vehicles

FLH Full Load Hours

GAMS General Algebraic Modelling System

GHG Greenhouse Gas

GHI Global Horizontal Irradiation

GSAM Generic Solar Ammonia Model

HB Haber-Bosch Synthesis Process

IEA International Energy Agency

ILR Inverter Load Ratio

IPCC Intergovernmental Panel on Climate Change

IRENA International Renewable Energy Agency

LBNL Lawrence Berkeley National Laboratory

LCOA Levelised Cost of Ammonia

LCOE Levelised Cost of Electricity

LHV Lower Heating Value

LNG Liquefied Natural Gas

LPG Liquefied Propane Gas

MILP Mixed Integer Linear Programming

MMBD Million Metric Barrels per Day

MMTPA Million Metric Tonne per Annum

Mtoe Million Tonne of Oil Equivalent

MTPD Metric Tonne per Day

NER Northeastern Region

NHM National Hydrogen Mission

NISE National Institute of Solar Energy

NIWE National Institute of Wind Energy

NR Northern Region

NREL National Renewable Energy Laboratory

OXGATE Oxford Green Ammonia TEchnology research group

PEMFC Proton Exchange Membrane Fuel Cell

PtX Power-to-X

RFP Request for Proposals

RICE Reciprocating Internal Combustion Engine

ROA Risk Opportunity Analysis

SCR Selective Catalytic Reduction

SMR Steam Methane Reforming

SOFC Solid Oxide Fuel Cell

SR Southern Region

SSRD Surface Solar Radiation Downward

TCO Total Cost of Ownership

TERI The Energy and Resources Institute

TMY Typical Meteorological Year

TRL Technology Readiness Level

V2G Vehicle to Grid

VRE Variable Renewable Energy

WACC Weighted Average Cost of Capital

WR Western Region

WY Weather Year

Notation

C_t = Investment expenditures in year t

A_t = Ammonia produced in year t

E_t = Electricity produced in year t

$O\&M_t$ = Operations and maintenance expenditures in the year t

n = economic lifetime of the plant

r = Weighted average cost of capital (WACC)

ΔH_{rxn} = Enthalpy of reaction

(u =) Wind speed in the eastward direction

(v =) Wind speed in the northward direction

V_z = Wind speed velocity to be calculated at height z

z = height above ground level for velocity v

z_{ref} = reference height where reference velocity is known

z_0 = roughness length in the current wind direction, 0.03 for open agricultural land

1 | Introduction

1.1 Thesis Overview

This thesis aims to answer the core research question: which significant roles will green ammonia have in decarbonised electricity systems? Currently, there are many gaps in understanding the roles of hydrogen and its derivatives, like ammonia. Therefore, this research's main objective is to identify the key roles and quantify the impact under various plausible scenarios. This research is highly relevant in an era of rapid transition in energy systems and specifically electricity grid systems, which will be the backbone of decarbonised energy systems of the future. Several modelling frameworks are developed in this thesis which culminate in novel energy system modelling, which is used to explore future pathways and to quantify the potential of this green fuel as compared to other technologies. An in depth case study on India's national electricity grid to 2050 is conducted to quantify the roles of ammonia in a highly relevant and illustrative context.

The roles of green ammonia in decarbonised electricity systems can be split into two categories: green ammonia production (Power-to-Ammonia) and re-electrification (Ammonia-to-Power). These two categories are represented in two research sub-questions, with a third sub-question probing into a key sensitivity factor affecting both power-to-ammonia and ammonia-to-power categories. The research sub-questions are:

1. Should green ammonia be used for re-electrification in power grids? How does using green ammonia for dispatchable power generation compare with traditionally modelled low-carbon technologies for dispatchable power, such as fossil fuel with Carbon Capture and Storage (CCS), nuclear energy, and bioenergy with or without CCS?

2. What are the effects of "sector coupling" green ammonia production (for various non-power sector users such as maritime shipping fuel and fertiliser) with the electricity grid system? Should green ammonia production be grid connected or islanded?

3. What are the effects of grid resilience on both potential roles (power-to-ammonia and ammonia-to-power), as explored via seasonal and interannual variation of solar PV and wind energy?

1.2 Map of the thesis

The thesis is structured to tackle these sub-questions with various relevant modelling methods, including chemical engineering, techno-economic, and energy system modelling techniques.

Chapter 1, this introductory chapter, provides historical and technical background and introduces the current context of green ammonia globally and in India. The motivations for the research and research questions are also highlighted.

Chapter 2 conducts a literature review of the relevant fields and highlights the gaps in the research around integrating ammonia into an Energy System Model (ESM) and in the foundational modelling steps preceding ESM integration. The literature review covers the relevant disciplines of power-to-ammonia modelling(Levelised Cost of Ammonia (LCOA) modelling), ammonia-to-power modelling (Levelised Cost of Electricity (LCOE) modelling), and sector coupling and energy system modelling.

Ultimately, to answer the research questions, a highly spatially and temporally granular ESM of an electricity grid with novel ammonia and hydrogen sector coupling is needed. This ESM is detailed in Chapters 4 and 5; however, several sub-models and higher level analysis are first needed as building blocks for this complex ESM. These building blocks are developed in

Chapter 3.

Chapter 3 also begins to shine a light on sub-question 1: “Should green ammonia be used for re-electrification in power grids?” To address this question and to compare ammonia-to-power with other competing technologies, an LCOE analysis is required. This LCOE in Chapter 3 is a first pass; to properly address sub-research questions 2 and 3, a highly detailed ESM is needed, as detailed in Chapters 4 and 5.

Chapter 4 delves into the state-of-the-art energy system modelling and how this thesis builds upon "traditional" approaches to modelling energy systems to answer sub-research questions 1, 2, and 3. Novel methodology of wind and solar multi-year profile generation is developed to address research sub-question 3 and the role of ammonia in providing grid resilience.

Chapter 5 highlights key results of applying the novel ESM methodology to a case-study of India and includes additional input assumptions to an ESM of India, such as the sectoral level forecasts of steel, fertiliser, transport, and maritime fuel in India.

Chapter 6 discusses the main findings and the implications for policymakers and businesses that are navigating the energy transition.

Chapter 7 concludes the thesis by answering the core research question and sub-questions, and outlining future directions of research based on this DPhil.

1.3 A brief introduction to green ammonia

1.3.1 The promise of hydrogen and ammonia

Carbon-free chemical energy storage technologies such as green hydrogen and green ammonia have been recognized as essential technologies for achieving net-zero greenhouse gas emissions

[23]. These energy dense fuels will play crucial roles in decarbonising heavy-duty transport (i.e., trucking, aviation, and shipping), decarbonising industrial processes such as fertiliser and steel production, providing long-duration storage and dispatchable electricity generation, and trading energy and hydrogen between regions [24]. Net-zero targets have been set by over 130 countries to date [25] and hydrogen specific roadmaps, strategies, and policies 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 [26, 27].

While hydrogen has experienced previous hype cycles and is more widely researched, the current flurry of targets and investments is also focusing on ammonia for the first time and its unique role in mitigating significant CO_2 emissions. Decarbonising ammonia is essential foremost for the existing uses of circa 180 Million Metric Tonne per Annum (MMTPA) of ammonia used predominantly for nitrogenous fertiliser. Nitrogenous fertiliser is key for feeding the global population, and although there is important research ongoing to improve fertiliser application efficiency and to reduce inorganic fertiliser applications, the long-term forecast to 2050 is still a growing ammonia demand of 23% to 37% from today's levels to produce fertiliser for a growing population [28]. Secondly, low-carbon ammonia is the leading candidate for replacing fossil fuel-based maritime shipping fuels [3]. The International Energy Agency (IEA)'s most recent estimates are that at least 45% of shipping fuel will be ammonia by 2050 in their net-zero scenario [27], while other projections by institutions like Lloyd's Register are up to 100% of shipping fuel by 2050 [29]. Considering these two sectors alone, green ammonia has mitigation potential of circa 5% of global Greenhouse Gas (GHG) emissions split between fertilisers (c. 1.8% of GHG emissions [1]) and shipping fuel (c. 2.9% of GHG emissions [30]). This is in agreement with IRENA's estimate that hydrogen and its derivatives will mitigate

10% of CO_2 emissions [21]. The final category of significant GHG mitigation potential for ammonia is via storage and trade of energy and hydrogen. The International Renewable Energy Agency (IRENA) estimates that half of all international trade of hydrogen in 2050 will occur as ammonia [21]. This stored or traded ammonia may be used as a fuel for dispatchable power [31] or cracked and used to deliver hydrogen to different end users [21]. The emissions reduction of this end use case is more difficult to estimate, and indeed the outcomes of this thesis shine a light on some of this potential. Even without putting a mitigation potential estimate to this last use case, at least 5% of GHG emissions mitigation potential from this one chemical is a significant role in the decarbonisation transition. The existing and new use cases of green ammonia, along with a general block flow diagram of a simplified production process are highlighted in Figure 1.1.

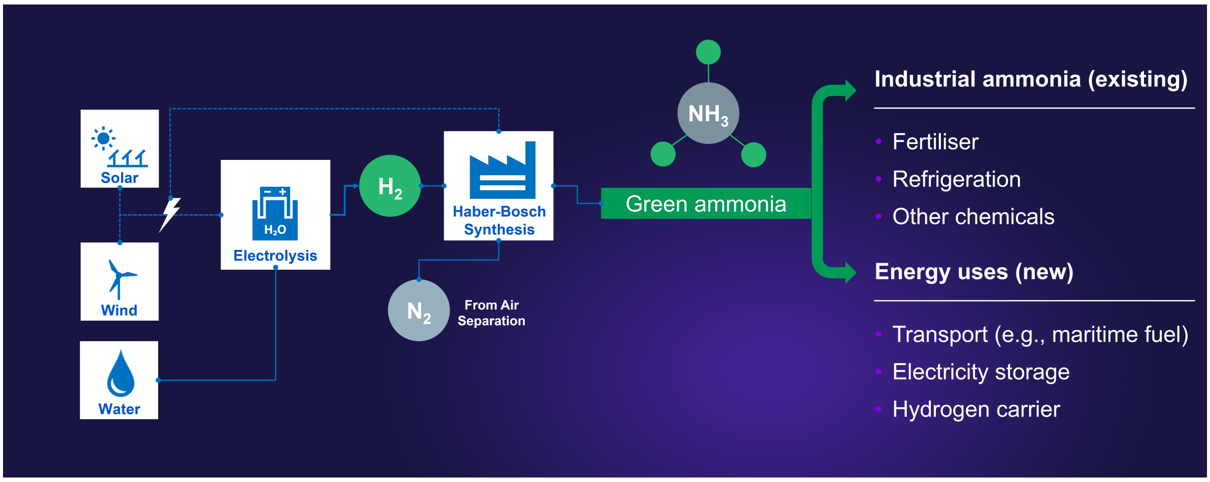


Figure 1.1: Overview of a simplified green ammonia production process from solar and wind electricity, and various existing industrial and energy demands for ammonia.

Two factors which differentiate this hype cycle from previous ones are the urgency of emissions reductions and the favourable economic situation of solar and wind power relative to fossil fuels. These factors, alongside others, are contributing to many announcements of industrial scale green hydrogen and projects to be commissioned in the coming years. Secifically, green ammonia production is being developed in all parts of the world: North America [32], Europe

[33–37], South America [38, 39], Oceania [40, 41], the Middle East [42], Africa [43], and Asia [44]. The pipeline of announcements is still accelerating for both hydrogen and ammonia. In 2019, the pipeline of low-carbon hydrogen was 2.3 MMTPA to 2030, which increased three-fold to 6.7 MMTPA by the end of 2020 [45]. Interestingly, at the end of 2019, there were only two demonstration scale projects operating in the world for green ammonia (in Oxford [46] and in Fukushima [47]) and only one publicly announced pre-commercial green ammonia project, in South Australia [48]. By early 2022, there are dozens of green ammonia projects in the pipeline.

1.3.2 A historical perspective

One reason for the rapid uptake of green ammonia production is the historical maturity of the production, storage, transport, and cracking technologies. Fundamentally, replacing fossil-fuel based production with green production requires substituting hydrogen production from Steam Methane Reforming (SMR) or coal gasification with water electrolysis powered by renewable electricity. The Haber-Bosch synthesis process can remain largely unchanged in the fossil-based design versus the green process; however, more flexibility in the ramping and minimum load level of the process are important to economically match the variability of renewable electricity and reduce costs.

The concept of producing *green* ammonia using hydrogen sourced from the electrolysis of water is not new– there have been several hydropower-based electrolysis facilities in the 1950s to 1990s used to make ammonia. Facilities were built and operated in Canada, Chile, Egypt, Iceland, India, Norway, Peru, and Zimbabwe [49]. These included Yara's facility in Glomfjord, Norway, until 1991, when natural gas availability and SMR eliminated the competitiveness of this method [50].

However, green ammonia has experienced a conceptual renaissance since the mid-2010s [51, 52] as two macro-trends became clear: first, the imperative to decarbonise *all* parts of the economy, and second, the rapid decline in wind and solar power costs and, thus, the reduced production cost gap between green ammonia and existing fossil fuel based ammonia production. Importantly, the renewed interest in decarbonised ammonia extended beyond existing fertiliser uses into energy-related applications. The concept for energy storage was more widely introduced via the seminal work from the Oxford Systems Engineering group, the Smith School of Enterprise and the Environment, the Oxford Chemistry Department, and Siemens in looking at green ammonia Levelised Cost of Ammonia (LCOA) via a process level design in *Analysis of Islanded Ammonia-Based Energy Storage Systems* (2015) [52]. As an outcome of this work, the Siemens Green Ammonia Demonstrator was built and commissioned in June 2018 as the first round-trip demonstration of green ammonia for energy storage (Power-to-Ammonia-to-Power) [46] (Figure 1.2).

The maturity of the entire end-to-end chain (i.e., production, storage, transport, cracking, combustion) of green ammonia is one of the major advantages in its adoption compared to other emerging technologies which compete in similar energy use-cases, specifically liquid hydrogen. First, nearly 60 countries from all geographies and income levels currently produce ammonia for fertiliser and chemicals, ranging from China, Russia, USA, UK to India, Trinidad, and Egypt [53]. At 180 MMTPA, ammonia is one of the most industrially produced chemicals in the world, accounting for one fifth of chemical sector energy demand [28]. Fundamentally, the Haber-Bosch ammonia synthesis process is over 100 years old, and the industrial know-how is widespread across the globe.

Secondly, ammonia is easily stored in large quantities at very low cost as a liquid in above-ground tanks, using mild pressure (10-20 bar), mild refrigeration (-33C), or a combination of

Figure 1.2: Power-to-ammonia-to-power demonstrator built at Rutherford Appleton Laboratory in Oxfordshire, UK as a collaboration between Siemens, University of Oxford, Cardiff University, and the Science and Technology Facilities Council (STFC). The system includes wind power, electrolysis, air separation via PSA, Haber-Bosch ammonia synthesis, ammonia storage, and ammonia / hydrogen combustion in a reciprocating engine.

both [54]. Large-scale, refrigerated liquid ammonia storage tanks have a capacity range from 4,550 to 50,000 tonnes [54]. Tanks are used all over the world, both in industrial and commercial settings. For example, the state of Iowa in the USA has almost 1 MMT of ammonia storage in tanks dispersed around the state for agricultural uses [55].

Thirdly, ammonia is transported around the world in large quantities via pipeline and via ship. Global infrastructure includes thousands of kilometres of pipeline, mainly in the USA (3,000 km, 2.9 MMTPA) and Russia (2,400 km, 3 MMTPA) [54]. Import and export terminals for ammonia already exist at most major ports (see Figure 1.3) [1]. A fleet of over 65 tankers enable overseas trade of 20 MMTPA of ammonia [56]. Furthermore, there is a potential to utilise many additional tankers that are compatible to either ship Liquefied Propane Gas (LPG) or ammonia. Therefore, there are a large body of existing assets which can transition to ammonia as LPG shipment reduces during the energy transition.

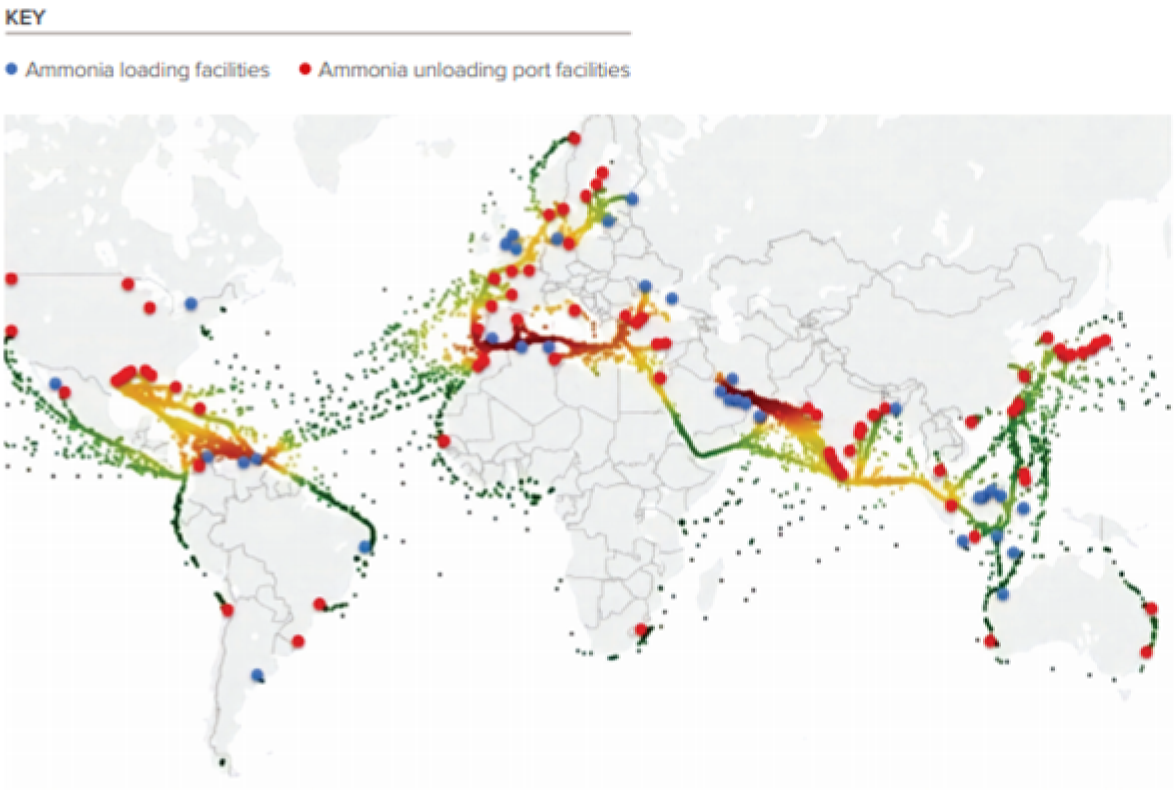


Figure 1.3: Ammonia import and export terminals with shipping heatmap, from [1]

Cracking ammonia is performed today at small scale for process forming gas in industrial processes, such as metal annealing [57]. In the past, large-scale cracking was used to generate nitrogen and hydrogen for industrial processes, including for operations at ammonia synthesis plants, with chemical companies claiming more than 30 years of operation of these plants [58]. While this technology went out of date due to cheaper alternatives, the core technology is mature and well-understood.

Finally, combustion of ammonia has been used in historical contexts, such as for powering buses in Belgium during World War II [50]; however, it is one of the less mature elements of the end-to-end chain due to the lower costs of fossil fuels for combustion technologies. Still, engine manufacturers such as MAN Engines and Mitsubishi have made clear targets to have ammonia compatible combustion engines on the market by 2024 and 2025, respectively, signalling the relative maturity of ammonia combustion [59, 60].

All of this mature infrastructural know-how is markedly different to other chemicals, especially the other leading candidate in many use-cases: liquid hydrogen. Liquid hydrogen only benefits from a global production capacity of 0.1 MMTPA [61], largely for niche uses like supplying NASA spacecraft fuel. Building efficient liquefaction industrial know-how will take many years, while ammonia production has a significant head start with existing production in every part of the world. Storing liquid hydrogen at -253 C is also very expensive, with very little installed storage to date (again, dominated by NASA) [62]. Finally, in shipping, the first liquid hydrogen tanker has just recently been built in 2021, but is only capable of transporting 90 tonnes of liquid hydrogen from Australia to Japan [63]. It will require a significant ramp up of ship building, port infrastructure and safety procedures, and liquefaction capability to come close to the 20 MMTPA of ammonia shipped today.

In summary, the historical perspective on green ammonia highlights that green ammonia can scale to the massive quantities and global infrastructure required to replace coal, oil and gas in the next decades. This point is somewhat captured in techno-economic analyses, via mature cost forecasts; however, it really does shift the dialogue from green ammonia as a theoretical solution to various decarbonisation challenges into a category of one of the few mitigating technologies which is actually capable of achieving meaningful GHG reduction in the coming decades. Moreover, the *faster* a transition to net-zero occurs, the *more* relevant the role of ammonia will be, due to this existing know-how and infrastructure compared to some of the other competing technologies which require further technical development and dissemination of industrial know-how from niche industries in few countries.

1.3.3 Health and Safety Considerations of Ammonia

Today, ammonia is safely handled in many industrial and agricultural environments around the world. While safe practices for bulk ammonia storage, transport, and use exist today, ammonia does have corrosive and toxic characteristics that warrant careful health and environmental procedures and caution.

From a health perspective, relatively small concentrations of ammonia are toxic. The toxicity depends on dosage and exposure type, but it can be dangerous to come into contact with ammonia via inhalation, skin or eye contact, or ingestion. At ambient temperatures and pressure, ammonia is a pungent, colourless gas. Breathing in low levels of ammonia may cause irritation to the eyes, nose and throat. Smelling salts are a tool used to release small concentrations of ammonia into airways and cause a strong physical reaction which wakes up an unconscious person. While small concentrations are irritating, high levels of ammonia may cause burns and swelling in the airways, lung damage and can be fatal. The recommended exposure limit for an 8 hour workday is 25 ppm, and short term exposure limit for 15 minutes is 35 ppm from the USA Occupational Safety and Health Administration [64]. Ammonia is readily detected by human sense of smell at concentrations around 10 ppm, below the levels that are harmful to health. Its characteristic smell is also found in common household cleaners. Ammonia is also found in nature, as it is produced from bacterial processes when plants, animals, and animal wastes decay.

Regarding environmental impact, ammonia itself is not a greenhouse gas, however it does decompose to NOx (a potent greenhouse gas) in the atmosphere. Today, only 20% of the ammonia used in agriculture is taken up into food and the remaining 80% runs into water, soil, and air [1]. Therefore, current agricultural practices require management of ammonia release to the environment. Ammonia and phosphorus runoff from agricultural practices causes eutrophication of bodies of water, leading to harmful algal blooms which kill fish and decrease aquatic life [65].

In the context of this research, emissions can be completely controlled when using ammonia for energy purposes. Detection can be more closely controlled than, for example, natural gas, and no venting or flaring are essential parts of the process of using ammonia for energy. There is more of a risk of increased global NOx emissions in using ammonia for energy purposes rather than ammonia emissions. Generating energy from ammonia involves converting ammonia back into nitrogen and water. This can either be done by first splitting ammonia into hydrogen and nitrogen and then converting hydrogen to water, or directly via converting ammonia to nitrogen and water. Chapter 2 includes further literature review around ammonia-to-power configurations. In an case of combustion (either of hydrogen from cracked ammonia or of direct ammonia combustion), NOx formation is likely in current combustion systems. For hydrogen, high temperature combustion of hydrogen in air leads to NOx formation. For ammonia, NOx can be formed both from fuel bound nitrogen along the combustion pathway as well as from high temperature reaction with the combustion air. Since ammonia does not have a very high flame temperature, temperature driven NOx is less likely in ammonia combustion than in fossil fuel combustion or hydrogen combustion. Fortunately, existing post-combustion technology, such as selective catalytic reduction (SCR), can be used to reduce NOx to nitrogen and water if NOx emissions are generated from an ammonia or hydrogen combustion system. Moreover, the existing SCR process, which is often used for scrubbing NOx emissions from diesel engines, actually utilises ammonia (or derivatives such as urea) as the chemical reducing agent. The current research in both hydrogen and ammonia combustion is focusing on designing NOx free combustion; however even if it takes some years of combustion research to eliminate NOx formation, the SCR process for NOx clean up already exists and is very low cost and mature.

In summary, ammonia is a substance that needs careful handling and environmental procedures. Fortunately, these procedures already exist around the world and are well practiced. Unfortunately, the health and safety qualities of ammonia do limit the usefulness of the chemical to controlled settings with trained operators, such as in power plants, on industrial ships, and in other industrial settings. This thesis focuses on use cases of ammonia where the health, safety, and environmental impact can be managed in an acceptable and climate friendly manner.

1.3.4 Colours of ammonia

Like hydrogen, ammonia is generally classified as grey (based on natural gas), brown or black (based on lignite or bituminous coal), blue (based on natural gas with Carbon Capture and Storage (CCS)), turquoise (based on methane pyrolysis), or green (based on water electrolysis and renewable electricity). Green and blue ammonia are the only scalable, cost-effective solutions for low-carbon ammonia production. Grey and brown are clearly incompatible with emission reduction targets due to their high emissions. Turquoise ammonia has highly uncertain costs due to the relatively lower Technology Readiness Level (TRL) of the technology. Furthermore, turquoise ammonia is dependent on the sales price of carbon black, which has a current market an order of magnitude smaller than the theoretical output of widespread turquoise ammonia production, creating clear uncertainty in the turquoise ammonia business model [28].

This thesis focuses exclusively on green ammonia over blue ammonia for several reasons. First, there is a clear cost trajectory that suggests that green ammonia will be lower cost than blue ammonia in the 2030 time range [21, 45]. As the focus of this thesis is long-term energy system modelling and most of the capacity will come online after 2030, green ammonia is the more relevant technology to consider. IRENA currently forecasts two thirds of low-carbon hydrogen and its derivates to be green by 2050, with one third being blue[21]. Secondly, the residual emissions from blue ammonia are a concern—both from upstream fugitive emissions of natural gas in the supply chain and CO_2 emissions at the production site due to incomplete capture. Again, considering the long term and net-zero targets, blue is incompatible without CO_2 offsets, which further hurt the economic competitiveness of blue ammonia. Finally, this work focuses on India as a case study, where blue ammonia is contextually irrelevant. Domestic natural gas reserves are very small in India, and imported Liquefied Natural Gas (LNG) comes at a significant price premium, thus making green ammonia nearly more economical than unabated natural gas based ammonia today [2]. Additionally, CO_2 geological storage sites are likely to be small and distributed, making CCS prohibitively expensive in the Indian context [2].

1.4 Context of green hydrogen and ammonia in India

India is chosen as the case study in this thesis due to its globally unmatched demand growth in all three relevant sectors: electricity, green hydrogen (for steel and transport demands), and green ammonia (for fertiliser and shipping fuel demands). India is also pioneering in green hydrogen and ammonia focused policy. The Indian government announced a target to be Net-Zero by 2070 [66] 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 electrolysers and fuel cells through green hydrogen obligations in industrial production of materials such as fertilisers, steel, and petrochemicals [67]. The proposed green ammonia obligations in the fertiliser sector would drive the world's fastest national green ammonia build out. Today, India is the world's largest importer of ammonia, with imports equivalent to 1.3 billion USD [21], not including the LNG which is also imported to make ammonia in India [2]. This import dependence further underscores the political and economic motivations to rapidly shift towards domestic green ammonia production.

However, the transformation of the Indian energy system extends far beyond green ammonia for fertiliser, and thus creates an ideal case study on the cross-sector role of ammonia in decarbonised energy systems. The Indian economy is poised for rapid economic growth, rapid urbanisation, rapid industrialisation, and rapid decarbonisation– all at the same time. In the IEA's global models, 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 [68]. Unsurprisingly, the IEA has firmly stated, **"Whichever way the global energy economy evolves from here, India will be firmly at its centre"** (IEA, 2021) [68].

In the IEA's modelling, India's projected CO_2 emissions increase from 2.2 to 3.7 GT CO_2 per year, which offsets all of the European CO_2 decreases in emissions— all while India stays below the per capita average CO_2 emissions of the world today [68]. This forecasted increase in CO_2 emissions is primarily driven by industrial emissions (i.e., steel, cement, fertiliser) and transport, especially from diesel trucks, with oil demand rising from 4.7 Million Metric Barrels per Day (MMBD) to 8.7 MMBD, compared to a global consumption today of approximately 100 MMBD [68]. The industrial sector is forecasted to increase cement and steel production by several fold to meet the construction boom as 270 million people are added to urban populations by 2040, and millions of Indian households are financially able to buy appliances, air conditioning units, and vehicles [68]. This unprecedented urbanisation forecast is the equivalent of adding a city the size of Los Angeles each year from now until 2040 [68].

At first glance, these figures of demand growth can be overwhelming from an energy system decarbonisation perspective; however, the electricity sector outlook is more optimistic and can underpin the decarbonisation of all of the other sectors with a rapid ramp up of electrification and Power-to-X (PtX) technologies. Solar with several hours of battery storage is cheaper than new coal power plants in India and soon will be lower cost than pre-existing coal power (i.e., just the operating cost of the coal plant) [68]. Even in the most conservative IEA scenarios, India is forecasted to have 20% of globally installed solar PV and the largest utility scale battery fleet *in the world*, accounting for 30% of global capacity by 2040 [68]. With this rapid decline in costs of renewable electricity generation and clear trajectory towards a decarbonised electricity sector, the relevant policy questions in India around national decarbonisation are pivoting towards green hydrogen and ammonia and related challenges like grid reliability and resilience.

The decarbonisation scenarios in this thesis are compiled from other sectoral level research 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 1.4. At a global level, IRENA forecasts that the production of green hydrogen and its derivatives will use 30% of the total electricity demand in 2050 [21], which closely matches the 25% estimate for the Indian energy system in this thesis. The scale of this new electricity generation infrastructure for producing green hydrogen and ammonia is tremendous, with electrolyser-connected renewable generation capacity in India exceeding the UK's entire electricity system generation (circa 300 TWh in 2019) by the mid-2030s. In this scenario, green hydrogen production in India will surpass existing grey hydrogen by the mid 2030's. Corroborating this scenario, the Indian government has recently announced a target of 5 MMTPA of green ammonia by 2030 as part of the NHM [18], which is nearly as much as the 6 MMTPA of fossil fuel based hydrogen used today in India [2]. This decarbonisation scenario demand for green hydrogen and ammonia is split into ammonia for shipping fuel (11% of electricity consumption), hydrogen for steel (6%), hydrogen for heavy vehicle transport (3%), ammonia for fertilisers (3%), and hydrogen for refining (1%). This scenario may be conservative, as synthetic aviation fuel is not yet included in this modelling, which may increase green hydrogen demand in India by an amount equivalent to shipping. Additionally, the modelling underpinning these sector forecasts by TERI [2] does not assume 100% decarbonisation in these sectors by 2050, but rather 50% of steel, 60% of ammonia fertiliser, and 30% refining demand are met by green hydrogen, while the remaining production remains fossil fuel based.

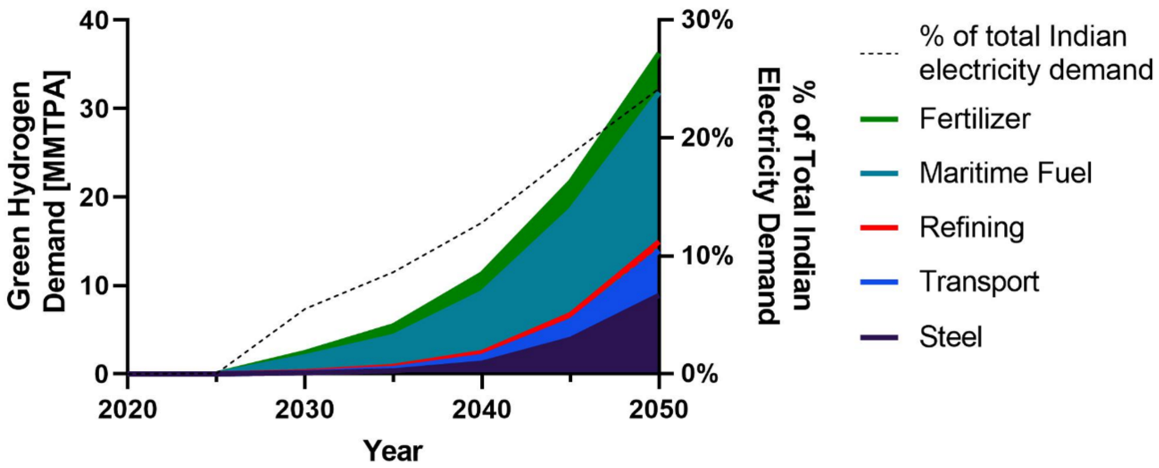


Figure 1.4: Green hydrogen and ammonia sector-level demand in India to 2050, including comparison to total final electricity demand (right axis). Main assumptions from TERI [2] for refining, transport, steel, and fertiliser and World Bank [3] for maritime fuel. See Chapter 5 for further information.

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 the pioneering policy of the NHM.

2 | Literature Review

2.1 Introduction

In this chapter, a literature review is conducted on the relevant fields of study, and the gaps are identified. There are three relevant general subject areas to review: (i) power-to-ammonia LCOA modelling, (ii) ammonia-to-power LCOE modelling, and (iii) ESM and sector coupling. Additionally, there is an India-specific ESM literature review (iv) to frame the context of the case study. The final section of this literature review chapter summarises the gaps across the literature and motivation for this research.

The significant gap that needs to be filled in order to answer this thesis's research questions is the gap in integrating ammonia into an ESM; however, to achieve this, the building block models of (i) and (ii) are needed, and indeed there are gaps in both fields of research that are highlighted in this section and needed to be filled in the process of building a ESM with deep ammonia integration.

2.2 LCOA literature review

Techno-economic modelling of green ammonia production is important for estimating accurate present and future LCOA. As a leading green fuel, the implications of these cost projections are similar to the effects of oil prices– the LCOA can affect numerous cross-sector systems, from shipping to agriculture, and it is important that projections are as accurate as possible for understanding the role of ammonia in decarbonised energy systems. In this section, a literature review demonstrates a split between "simplified" and "complex" methodologies for modelling

LCOA. Within both of these approaches, the strengths, weaknesses, and gaps are highlighted. The highlighted gaps are addressed in Section 3.2.

2.2.1 Simple LCOA calculations

Simplified methods of estimating LCOA are abundant in the literature, especially in high-level reports on broad subjects like *The Future of Hydrogen* [24] and decarbonising shipping [29, 69, 70]. These reports seek to approximate the LCOA in the future to compare costs against fossil fuel and green alternatives in sectors such as maritime fuel and nitrogenous fertilisers. To estimate LCOA, the models used in these reports use generic and oftentimes unjustified assumptions about key design input variables to create a simplistic view of the costs of a green ammonia synthesis plant. Two of the most commonly assumed dependent variables of simple LCOA equations are the Full Load Hours (FLH) and LCOE of the VRE (e.g., 7,000 FLH at $18-21/MWh [69], 3,000 FLH at $25-50/MWh [24], and 8,000 FLH at $43.2/MWh [70]). These models miss crucial design steps and fail to address fundamental questions about how their plant would even operate: how big should the electrolyser be for the IEA's supposed system [24] with 3,000 FLH of VRE at $25-50/MWh? What does the profile of the 3,000 FLH look like? What happens if there is a wind drought for two weeks? Does the plant just shut down? Are they assuming the Haber-Bosch plant can ramp down or deal with frequent shut-downs? If so, to what level? Why is no hydrogen storage considered, when surely there needs to be some? Unfortunately, these overly simple models design plants which are almost certainly technically infeasible and disproportionately sized, resulting in LCOA estimates that are far from the results of more detailed models. Not only does this simplistic approach distort the LCOA forecasts, these non-optimal or non-functional implicit plant designs also distort the sensitivity analysis and misrepresent future scenarios.

2.2.2 Complex LCOA calculations

Complex modelling of LCOA, on the other hand, starts with process level optimisation of equipment sizing to ensure feasible plant operation and optimised LCOA. This field of research has been led by the Oxford Green Ammonia TEchnology research group (OXGATE) research group [6, 71–74]. Nayak-Luke et al.[6] contend that determining LCOA to a useful accuracy and understanding key sensitivities requires techno-economic optimisation to the process level based on the specific geographical wind and solar supply profile and cost [6]. Other complex models following similar methodology have been published by Beerbühl et al. [75], Armijo et al. [76], and Fasihi et al. [77].

The process variable that largely necessitates complex modelling is the limited flexibility of the Haber-Bosch Synthesis Process (HB) loop, which is unable to mirror the incoming VRE profile. Plants in operation today do not have flexibility below 50-60% of minimum load [78] as the source of hydrogen to the process is fossil fuel based and thus the least cost strategy is to run 24/7 to maximise all assets' utilisation. 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 [78], 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 [79]. In complex LCOA modelling, process units are sized to manage the technical requirement of minimum HB load given the geographic specific solar and wind profiles while also minimising cost based on input cost assumptions. Simplified models do not consider HB minimum load, and thus do not consider the electrolyser over-sizing or curtailment which would significantly alter the electrolyser Capital Expenditure (CAPEX) and VRE LCOE. In complex models, the electrolyser is usually oversized to produce excess H_2, which is stored in H_2 storage, and then used during low RE for feedstock and electricity in order to maintain feasible operation.

Finally, the complex models scarcely consider grid connection, and have yet to consider the green ammonia production integrated flexibly with a grid that is also optimising in decarbonised generation and storage. The production modelling of ammonia is typically modelled in islanded systems [6, 75–77]. Salmon et al. [72] have pioneered in grid connected, flexible ammonia synthesis in an Australian grid context, but fail to consider the future developments on the grid, and rely only on present day time of use prices. Ikäheimo et al. [80] consider grid connected ammonia synthesis in a changing system over time, but do not consider any HB flexibility and thus build uneconomic plants which do not really explore the benefits of grid connection.

2.2.3 Gaps in LCOA modelling

There are two identified gaps in LCOA modelling: first, there is no simple methodology which is accurate and second, there are no LCOA models which consider grid connecting ammonia plants which are integrated into a larger electricity grid which is changing over time.

Clearly, simplified methods are not accurate for LCOA calculations because they are not designing functional plants; however, there are weaknesses in the complex methodology which somewhat restrict their utility. Complex models require geographic specific profiles of wind and solar resources and country specific equipment, labour, and financing costs. These models are "black box" optimisation models which lack transparency for the wider research community to define assumptions and reconfigurations. This inhibits the addition of new technologies such as solar PV with single axis tracking and rapidly falling prices of battery storage to the models, for example, without significant model development. A “simple” methodology is missing which can be widely applied to multiple geographies, and accurate (when compared to complex LCOA models). This research’s questions are not focused on calculating a global average LCOA per se, but are interested in general LCOE modelling of ammonia-to-power (sub-research question 1) which requires an input assumption for ammonia costs over time. Therefore, a simple, widely applicable, and accurate LCOA model would be useful for informing this research sub-question. Indeed, averaged literature values could have been used for input to the LCOE analysis, but this research found that creating a simple LCOA model was more defensible and allowed for insights into the sensitivities of this islanded LCOA baseline. The model created is detailed in Chapter 3.

Regarding the gap of grid integrated LCOA analysis which considers changing grids over time and flexible HB plants, a capacity expansion and operation dispatch electricity system model is needed to fill this gap. This model is detailed in Chapters 4 and 5.

2.3 Ammonia-to-power LCOE

Combustion of ammonia has been used in historical contexts, such as for powering buses in Belgium during World War II [50]; however, it is one of the less mature elements of the end-to-end chain of using green ammonia for energy applications. Due to this lower level of maturity, there is almost no literature on modelling LCOE of ammonia-to-power. The few examples from literature are reviewed and gaps are highlighted. Moreover, this section provides a literature review of the technological pathways for ammonia-to-power and the justification for focusing on re-electrification using gas turbines with various scenarios of pre-combustion ammonia cracking.

2.3.1 Technologies for stationary ammonia-to-power

Ammonia is increasingly being considered as a direct or indirect fuel for stationary power plants. Ammonia, and the hydrogen contained within ammonia, can be transformed into electricity via thermochemical routes (turbines or engines) or electrochemical routes (fuel cells). Additionally, ammonia can be decomposed or "cracked" back into H_2 and N_2 via endothermic decomposition in the presence of a catalyst (Equation 2.1) to feed hydrogen compatible power generation equipment, such as hydrogen fuel cells or hydrogen gas turbines.

$$2NH_3 \rightarrow 3H_2 + N_2 \qquad \Delta H_{rxn} = 92\frac{kJ}{mol} \tag{2.1}$$

The main technical pathways for transforming ammonia into energy are outlined in Figure 2.1. This thesis presents novel modelling on the gas turbine route, which is found to be the most economically competitive route in a high-level comparison (Cesaro et al. 2021) [73]. All routes are briefly explored from a technological level in this chapter.

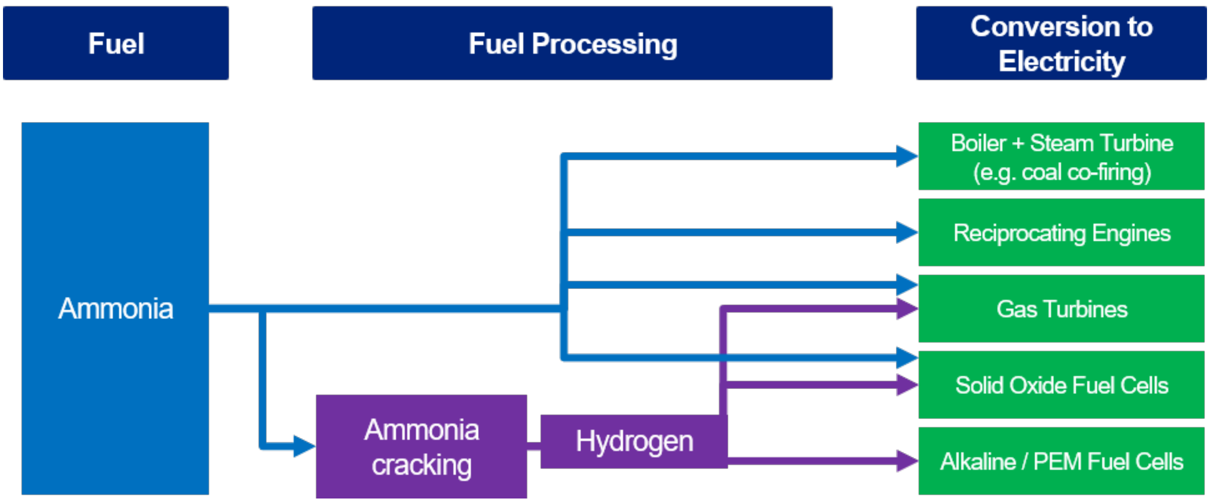


Figure 2.1: Overview of Ammonia-to-power pathways for generating power in stationary power plants

Co-firing ammonia in coal power plants

Ammonia co-firing in coal plants is seen as a method for reducing coal power plant emissions during their 50 year lifetimes, especially since over 1,250 GW of global coal plants will still have a lifetime of 20 years remaining in 2030 [24]. An upper blending ratio of 20% ammonia (by energy content) with pulverised coal has been demonstrated by IHI Corporation in Japan in 2018 to reduce emissions from 795 to 636 g CO_2/kWh [81]. Modelling suggests the burners of existing coal plants will not be able to burn higher blends of ammonia, as co-firing ratios of even 40% ammonia have significant quantities of unreacted ammonia slipping through the combustion step and being emitted through the exhaust [82]. Coal plants have lower efficiency than Combined Cycle Gas Turbine (CCGT) plants, with Japan having some of the highest coal plant efficiencies at 42% based on the Lower Heating Value (LHV) of the fuel [83]. Using these highly efficient coal plants and a steam coal price of 100 USD/t in Japan [84], the cost of this CO_2 offsetting is quite high at 200 USD/t CO_2 for a landed ammonia price of 400 USD/t. In comparison, the cost of CCS at a coal plant in Japan is estimated at 125 USD/t CO_2 [85]. Co-firing coal plants requires a green ammonia price at less than 300 USD/t to compete with fossil fuel with CCS.

Undoubtedly, there are more economical methods of avoiding CO_2 emissions than ammonia co-firing at coal plants; however, the Japanese government and industry seem intent on pursuing ammonia co-firing in the short-term as a stepping stone to 100% ammonia combustion in the long-term. Besides being technically unproven, this long-term goal would be a very expensive form of baseload power at a thermal efficiency of only 42%, whereas a CCGT would be more economical at a efficiency above 60%.

Ultimately, the motivation for the Japanese and other countries may be in utilising existing coal power plant assets, rather than a pure new-build LCOE analysis. The scale of CO_2 emission reduction from co-firing coal plants with ammonia, even at 20%, is massive if applied over all existing coal plants in 2030, totaling 1.2 Gt/year of CO_2 emissions avoided [24]. In short, the high cost may be justified as co-firing with ammonia offers a bridging technology to continue the use of existing assets. JERA, a coal power plant owner and operator in Japan, has recently announced a Request for Proposals (RFP) for 0.5 MMTPA supply of low-carbon ammonia from 2027 to the 2040s for coal co-firing, signalling clear intentions to proceed with the investigation of ammonia co-firing [86].

Fuel Cells

Proton Exchange Membrane Fuel Cell (PEMFC), Alkaline Fuel Cell (AFC) and Solid Oxide Fuel Cell (SOFC) technologies each have potential applications with ammonia.

PEMFC and AFC are fundamentally hydrogen electrochemical technologies and thus require cracking of ammonia back into hydrogen and nitrogen as a first step. PEMFC are generally used for transport applications, and not applicable for power plant stationary power due to the small scale, high capital costs at 1,300 USD/kW, and lifetimes of less than 10 years [87]. Furthermore, to use cracked ammonia to feed PEMFC, ammonia traces must be purified to under 0.1 ppm to adhere to the strict H_2 purity requirements for PEMFC, which is likely to add considerable costs. AFC are more tolerant to trace ammonia and have a lower cost; however, they have a large footprint requirement, and size is generally limited to less than 50 MW [24]. In smaller stationary power markets, AFC or PEMFC fueled with cracked ammonia may be competitive, as gas turbines are less competitive at these small scales. For example, AFC fueled with cracked ammonia may already approach cost parity to kW scale off-grid diesel generators in some markets due to lower maintenance cost and higher fuel efficiency. Off-grid telecom towers represent a large market of off-grid diesel generators, and at least two commercial entities, AFC Energy [88] and GenCell [89], are investigating the commercial potential of ammonia AFC off-grid telecom solutions. In Kenya, GenCell announced a commercial agreement in 2018 to power 800 off-grid telecom towers with AFC utilising an ammonia feedstock [90]. The 4 kW units from GenCell consume 2.5 kg NH_3/hr with an overall efficiency of 31% based on the LHV of ammonia, and a reported LCOE of 0.50 USD/kWh [89]. The fuel cost of ammonia at roughly 500 USD/t is equivalent to diesel fuel cost at 1 USD/l, assuming the same 30% fuel efficiency for both AFC with ammonia cracking and diesel genset, highlighting the potential economic competitiveness of ammonia for offgrid power applications [73]. Indeed, state-of-the-art mini-grid solutions are solar-battery-diesel hybrid systems, with an LCOE of at least 0.60 USD/kWh [91] and therefore AFC stationary power may compete in the emerging mini-grid market as well. The first solar-hydrogen off-grid project has been announced in Uganda for powering a mini-grid [92], whilst no projects including ammonia in rural mini-grids have been announced yet.

Directly using ammonia in SOFCs, or using a partially cracked stream of ammonia and hydrogen, is still in the research phase at kW levels [93]; however, ammonia SOFCs are being scaled for a 2 MW shipping project by 2024 [94]. More information is needed on the cost of SOFC; however, it is likely that the capital cost of SOFC will remain too high to compete in large stationary power for some years.

Reciprocating Engines

Ammonia is being investigated for combustion in Reciprocating Internal Combustion Engine (RICE) by ship engine developers, such as MAN Energy Solutions [59] and Wartsila [95]. RICE engines can also be used onshore for stationary power. For example, the largest RICE power plant uses 38 Wartsila multi-fuel engines for a combined 573 MW capacity, matching large gas turbine or steam turbine power plant output [96]. Another recent RICE plant uses

20 Jenbacher engines for a combined output of 190 MW in Germany, and other RICE power plants in the 50 MW range are becoming more common for distributed back-up and peaking power [97].

Some of the advantages of using RICE for power plants are the competitive capital cost, the resilience to frequent daily cycling (i.e., for peaking power plants), the multi-fuel capabilities, and the high open cycle efficiency [97]. Some of the disadvantages include frequent required shutdowns for maintenance, large weight and footprint of many smaller engines to achieve power plant scale power output, higher NO_X emissions, and higher noise. These engines are also the first movers towards ammonia, due to the relevance in the shipping sector, and therefore may be ready for spillover into the power sector quicker as well. According to MAN, the ammonia fed marine RICE is 95% similar to existing engines [59] and is usually quoted to have the same efficiency value of 50% [8]. While RICE are an important up-and-coming technology, especially for peaking power needs, the standard for large scale stationary power generation is turbine technology, and this thesis therefore most closely considers turbines for stationary power. Additionally, RE seasonality, which is a key research question of this thesis, is likely better met by gas turbines which have high reliability, lower maintenance, and lower costs when the use case is steadier, such as in a seasonal use-case. Although this thesis focuses on GTs, many of the findings in Chapter 6 would be applicable to RICE engines in place of CCGT, as the costs and efficiencies are fairly close.

Gas turbines

Hydrogen has been explored extensively as a carbon-free fuel for gas turbines in the power sector, with most manufacturers committing to 100% hydrogen compatibility in gas turbines by 2030 [98]. Mitsubishi has been awarded the first large contract for 840 MW of hydrogen compatible gas turbines operating at 30% H_2 in 2025 and 100% H_2 by 2045 [99]. Notably, this location in Utah, USA will utilise a large underground salt cavern for storage of hydrogen. Siemens Energy has announced a power-to-hydrogen-to-power storage system, equipped with electrolysers, hydrogen storage, and a 12 MW 100% hydrogen gas turbine by 2023 [100].

Recently, there has been a focus on using ammonia as a means to deliver these large volumes of hydrogen to gas turbines in locations without salt caverns. Salt caverns are geographically constrained, and have challenges with the rate of hydrogen withdrawal rates being limited to 6% to 15% of the storage capacity per day due to mechanical strength limits [101]. Siemens Energy's green ammonia white-paper (Cesaro, Wilkinson, & Eisfelder, 2020) [4], highlights the practical challenges of storing GWh of hydrogen compared to ammonia, as shown in Figure 2.2. This practicality translates to cost, as the cost of aboveground storage of hydrogen is over 100 times more expensive than aboveground storage of ammonia [73]. As corroboration of this push towards ammonia for gas turbines, Mitsubishi, on of the major gas turbine manufacturers alongside Siemens Energy and General Electric, announced in March of 2021 that they would have a 40 MW ammonia gas turbine run on the market by 2025 [60].

2.3.2 Ammonia-to-power standalone LCOE

To date, there are no known LCOE analyses of ammonia-to-power. Technological progress in ammonia-to-power has been extensively reviewed by [102] however no techno-economic analysis is included in the review. Wijayanta et al. [103] model hydrogen import to Japan in different carrier molecules, including ammonia with cracking, but stop short of modelling the re-electrification of the hydrogen, or comparing with other fuels.

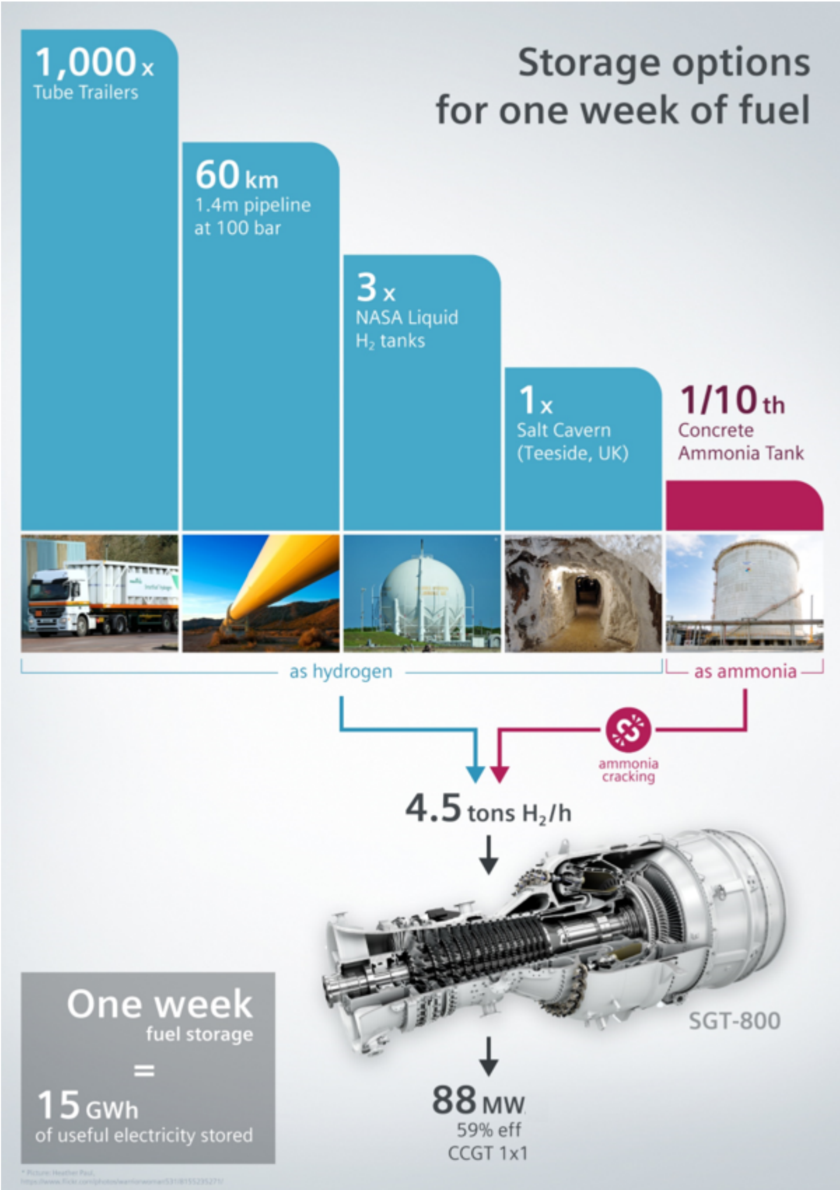


Figure 2.2: Comparison of one week of fuel storage for a mid-sized CCGT (88 MW) in the form of hydrogen in tube trailers, pipeline, liquid tanks, salt caverns, and ammonia. Graphic reprinted from [4]

2.3.3 Ammonia-to-power for dispatchable power in ESM

Furthermore, ESM studies based on VRE dominated systems have increasingly identified the need for long-duration storage [104] or firm generating capacity [105] for achieving zero emissions in the electricity grid. Many studies use significant nuclear and CCS technologies [23]; 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, as shown in the results of Chapter 3.

The few analyses that do include alternatives to nuclear and CCS technologies fall short of properly considering ammonia. Cole et al. [106] find a least-cost, 100% decarbonized USA grid deploys over 500 GW of green hydrogen-based electricity generation via gas turbines. However, Cole et al. [106] neither consider the practicality of storing all of this hydrogen, nor the potential of ammonia. Furthermore, it is quite astounding that Cole et al. [106] do not consider grid connected electrolysis for any sector coupling load-shifting– not even for the vast quantities of hydrogen consumed in the model itself. The only other ESM that has considered ammonia-to-power is Ikäheimo et al. [80]. Ikäheimo et al. [80] include ammonia-to-power via gas turbines as an option in their ESM of Northern Europe to 2050, but do not offer detailed justification of the capital costs or efficiency of their ammonia-to-power assumptions. Additionally, [80] do not report or compare ammonia-to-power on an LCOE basis with any competing technologies. Finally, Ikäheimo et al. [80] do not consider any ammonia synthesis flexibility, and thus miss the holistic sector coupling potential.

2.3.4 Gaps in Ammonia-to-power LCOE

First, there is a gap in the techno-economic comparison of green ammonia-to-power at power plant scale, especially compared with front-running low-carbon, dispatchable technologies such as fossil fuel with CCS, BECCS, and nuclear power. Within this modelling of ammmonia-to-power, there is a gap in modelling the comparison between various integrated cracking scenarios, i.e., whether the gas turbine is fuelled by pure ammonia, fully cracked to hydrogen, or a partially cracked mix.

Secondly, there is a gap in including power-to-ammonia and ammonia-to-power in an integrated, dynamic way with evolving electricity grids. ESM find a clear need for dispatchable technologies, but do not consider ammonia-to-power a potential technology. Furthermore, when they do include other synthetic fuels, they miss the sector coupling potential, as outlined in the next section of the literature review on sector coupling in ESM.

2.4 ESM and Sector Coupling Literature review

The complexity surrounding the analysis of a society's energy systems is magnified by systemic forces such as rapid electrification, industrialisation, decentralisation, decarbonisation, and high penetration of Variable Renewable Energy (VRE). ESMs are a key tool for providing insights into these complexities for research institutions, policy makers, and energy companies. Computational ESMs have been used for decades, dating back in the literature to the 1950s, when linear programming was first being used to optimise capacity expansion in electricity generation [107]. Some of the types of ESM used today include energy planning models, supply-demand models, forecasting models, renewable energy models, emission reduction models, optimisation models and new modelling techniques based on neural networks or fuzzy logic [22].

ESMs have been developed to investigate a range of research, industrial, and policy questions, and the choice of ESM depends on the question being asked. Different tools have different optimisation types, represent different sectors and have different time and geography aggregation affecting the areas of generation, transmission, flexibility, new investments, etc. No model covers all analyses, and models are constantly changing and expanding to cover different purposes. The ESM landscape, specifically the modelling of electricity systems, has been evolving in recent years as the energy sector undergoes massive disruption. One key trend in ESM is the focus on better representation of the integration of VRE, especially wind, solar PV, and batteries. Despite significant progress, there are still meaningful gaps in the modelling community relevant to this thesis, which are highlighted at the end of this section. This research's questions fit certain criteria, as it seeks to investigate incorporating an emerging technology (green ammonia) via sector coupling into future grids with high levels of VRE.

2.4.1 Energy System Modelling landscape

The number of models and model development activities have increased in recent years, and there are several reviews in the literature analysing and categorising different ESM to allow researchers to match their specific research question to an appropriate model. Connelly et al. [108] provided an analysis and differentiation of 37 prominent ESMs used specifically for modelling VRE integration (including Balmorel, the model chosen for addressing this research question). More recently, Hall and Buckley [109] review 22 ESM used in the UK, and Ringkjob et al. [22] review 75 ESM specifically for electricity systems, including Balmorel. Due to the more comprehensive and recent review in Ringkjob et al. [22], their framework is used in this thesis for classifying and selecting an electricity system model, with the criteria outlined in Table 2.1. Additionally, the 17 criteria used in [22] are very similar to those used in [108] and [109].

First, ESM can be categorised by the *purpose* (Investment decision support, operation decision support, power system analysis tool, scenario, or hybrid), *approach* (bottom up, top down, or hybrid), and *methodology* (simulation, optimisation, equilibrium, or hybrid). As a *purpose*, some models investigate capacity planning investment decisions over time, planning for future changes to the generation supply, demand, transmission grid, energy storage, etc. Operational decision support models investigate topics like dispatch planning for a grid. Power system analysis tools are similar to operational decision models but are looking at a smaller

Criteria	Description / options	Criteria for this research
Purpose	Why is the research question being addressed? Models can fit into multiple categories: Investment Decision Support, Operation Decision Support, Scenario, Power System Analysis Tool	Investment Decision Support & Operation Decision Support
Approach	Bottom up (many technologies included) and/or top down (macroeconomic view of energy demand and supply). Or hybrid.	Hybrid
Methodology	Simulation, optimisation, scenario, and/or equilibrium.	Optimisation, Scenario
Spatiotemporal parameters		
Temporal resolution	Milliseconds to decades. Timesteps can be fixed or a user input.	Hours, Weeks (Seasons), Years
Modelling Horizon	Milliseconds to decades	30 years (2050)
Geographical coverage	Individual units, mini-grid, local and district, state, national, international, global.	State, National
Techno-economic parameters		
Conventional Generation	Thermal, nuclear, bioenergy power plants, either individually or aggregated	All (which are relevant for case study)
Renewable Generation	Can include hydro (reservoir, run-of-river), solar PV, solar thermal, wind (onshore, offshore), geothermal, tidal, etc. VRE data can use historical meteorological data at small timesteps or average capacity factors, or can use stochastic methods.	All (which are relevant for case study)
Storage	Pumped hydro, batteries (of various types), compressed air energy storage, hydrogen and other chemical storage	All, including power-to-ammonia-to-power
Grid	Very detailed (stability, short circuit analyses, harmonics, etc.), or regional flows (using e AC (alternating current) flow, DC (direct current) flow or by net transfer capacities (NTC).	Regional flows in simple manner (NTC)
Commodities	Electricity, liquid fuels, natural gas, heat, hydrogen, etc.	Electricity, hydrogen, ammonia
Demand Sector	Separate (e.g. Buildings, industry, agriculture, transport, etc) or aggregated.	Aggregated
Demand elasticity	Elastic (the demand will change with price fluctuations) or inelastic (demand will not change with price fluctuations)	Inelastic (the complexity in elastic is not the focus of this work)
Demand Response	If included, Demand response can be modelled as a negative storage or negative generating unit, or shifting unmet flexible loads to following timesteps.	Flexible hydrogen and ammonia synthesis, but demands do not have to be responsive (i.e., demands can be fixed)
Costs	Investment (CAPEX), fixed and variable operation & maintenance, fuel, CO2, taxes, balancing costs (start-up, shut-down and ramping costs), etc.	All power plants costs, including CO2 taxes. Balancing costs nice to have, but not essential as they increase the calculation time
Market	Electricity market (balance supply and demand), reserve market, capacity market, no market	Electricity market
Emissions	CO2, NOx, SOx, CH4, etc. or CO2 equivalent	CO2 equivalent

Table 2.1: Criteria from Ringkjob et al.[22] and the relevant categorisation of this thesis's ESM

scale system, such as a single wind turbine and the power flows to and from the unit. Finally, scenario models look at various long-term scenarios and often are used to investigate the potential effects of policies. The *approach* distinction refers to whether the model uses detailed technical aspects of the energy system (bottom up) or a top down, macroeconomic approach to the model. The *methodology* can be an optimisation (often based on cost), a simulation (based on governing equations and relationships either at a system level or agent level), or equilibrium (based on economic modelling of the wider economy beyond the electricity sector). In all three categories, hybrid options are models that fit into two or more of the categories.

Beyond these three categories, the other two broad categories of classification are the *spa-*

tiotemporal range of the ESM and the *techno-economic* considerations of the ESM. *Spatiotemporally*, some models are used to answer very temporally and spatially granular topics such as micro-grid operations and sub-second grid inertia, to temporally and spatially vast questions such as country scale energy transitions to net-zero over decade long timesteps. Finally, models differ in technological and economic (i.e., *techno-economic*) factors such as which technologies are included in the model, which demand sectors are included, if demand side response or demand flexibility are included, which costs are included (such as CO_2 costs or ramping costs), which markets are modelled (such as the electricity market, reserve market or balancing market), and emissions. Ringkjob et al. [22] find that most of the 75 models reviewed are bottom-up optimisation models which have the purpose of giving investment and/or operation decision support, which indeed is in line with the requirement for this thesis's research questions.

2.4.1.1 General ESM limitations and gaps

In general, most questions on energy systems can be addressed using one or more of the available suite of models. However, models have limitations and several common limitations across the suite.

First, the temporal resolution is a challenge for modelling VRE integration, as wind and solar PV resources are variable at very small timescales as well as wind power cycles at longer time scales beyond years. Significant work has been directed toward calibrating low temporal resolution models which might only have several time slices per year, with higher temporal resolution models using sub hourly modelling or employing calculation-time intensive unit commitment. Despite attempts at calibration, low temporal resolution models are still found to incorrectly estimate the generation of VRE and thus underestimate the required investments in the system to manage the variability [22].

Second, the flexibility on the demand side of the future energy systems is still in nascent stages of being modelled. This extends from individual prosumers making more decisions in the system to large scale industrial demand flexibility. Third, the sector coupling of heat, transport, and industry to the power sector are also still overlooked in most models. This simplification is increasingly misrepresentative as the sectors become intertwined via electrification and hydrogen, as discussed in the next section. Fourthly, impacts beyond the electricity system are increasingly relevant, like effects on water and food systems, life-cycle-analysis-based modelling, land use changes, labour changes, etc. Yet the models are largely missing these other segments of the real-world effects of the ESM.

Fifthly, validation is a challenge with most modelling. For some of the power system analysis tools, real world data can validate the models. However, for future planning models, the uncertainty is very large and it is effectively impossible to correctly predict external disruptive events, like wars and new technological breakthroughs. Additionally, the effects of climate change are not well represented in the modelling, such as changes to wind resources to changes to demand due to increased temperatures.

In this thesis, an ESM is selected from these reviews for its applicability to answer the research questions. The selection process is outlined in Chapter 4, based on the Ringkjob et al. [22] classification in Table 2.1. Beyond selecting an appropriate ESM, three new modelling methodologies are added to this “standard” ESM to address several of these limitations listed above, at least partly, and fill gaps in the ESM literature. The next section expands upon the third general gap in the ESM literature highlighted above: sector coupling of hydrogen and ammonia, as it is the key gap which is identified and filled in this thesis and warrants a deeper deep dive into the state-of-the-art and gaps in the literature.

2.4.2 Sector coupling in ESM

2.4.2.1 Terminology

The definitions around sector coupling and related terms (e.g. power-to-X, multi energy systems) are still shifting as technologies develop and consensus varies around the concepts. For this work, sector coupling is defined as the coordinated operation and planning of several systems together [110]. While there are examples of sector coupling which do not involve the electricity grid (e.g. waste heat from industry used to heat homes via district heating networks), the focus for this thesis is on sector coupling which interacts with the power sector, i.e., the electricity grid. Electricity grid sector coupling accounts for most of the sector coupling literature, as the energy transition trend is generally towards electrification of all sectors and electrolytic production of hydrogen for indirect electrification.

The most relevant sector coupling concepts can be divided into sector couplings between the power sector and three other sectors as shown in Figure 2.3.: (i) electric transport sector coupling, such as smart charging of EVs and vehicle to grid discharging, (ii) thermal sector coupling such as load shifting of residential and industrial heating and cooling demands as well as waste heat from industry with district heating, and (iii) chemical sector coupling, which includes PtX concepts for use in fertiliser, steel, transport (synthetic hydrocarbons and other e-fuels) and re-electrification.

Power-to-X is a related concept, but can be considered to include strictly the conversion step to something non-electrical, and therefore does not capture the full sector coupling concept (e.g. power-to-X-to-power or power-to-X-to-heat). The most relevant concepts in PtX can be split

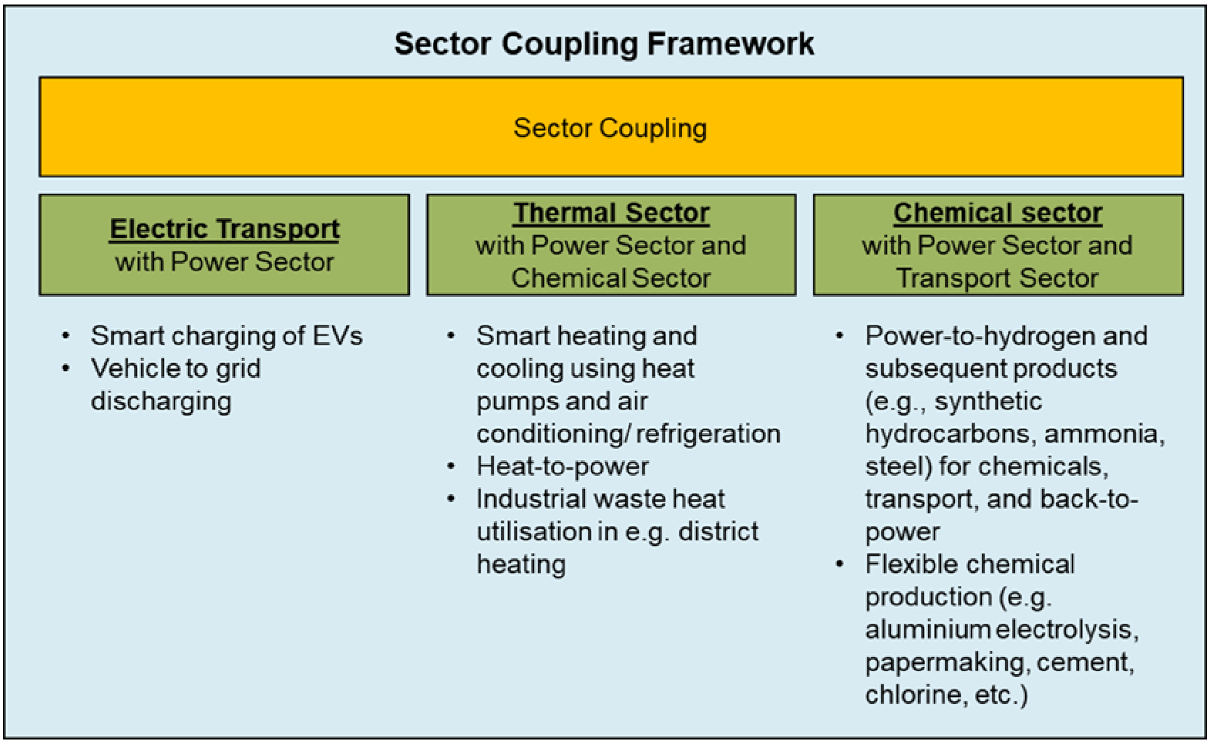


Figure 2.3: Conceptual overview of frequently discussed concepts which fall under the sector coupling umbrella, divided into the Transport, Thermal, and Chemical sectors, with the Power Sector as the foundation. Note: by definition, there are relationships between sectors for each of the examples, and thus they are not necessarily mutually exclusive to one of the three headers but organised as such for simplicity.

into power-to-hydrogen and power-to-heat, as shown in Figure 2.4. Power-to-hydrogen then can be further subdivided to power-to-gas (hydrogen, synthetic methane) and power-to-liquids (synthetic hydrocarbon fuels, usually not including ammonia) and power-to-chemicals [5].

The PtX framework generally does not explicitly cover power-to-commodities, such as paper, steel, aluminium, cement, chlorine, fertilisers, etc. which also have sector coupling potential via demand side response and load shifting [110]. Arguably they may be made up of some intermediates, such as hydrogen and heat, but, like synthetic methane in power-to-gas, it is sometimes more useful to identify the final "X" than the intermediates (i.e., power-to-methane could be covered by power-to-hydrogen and power-to-CO_2).

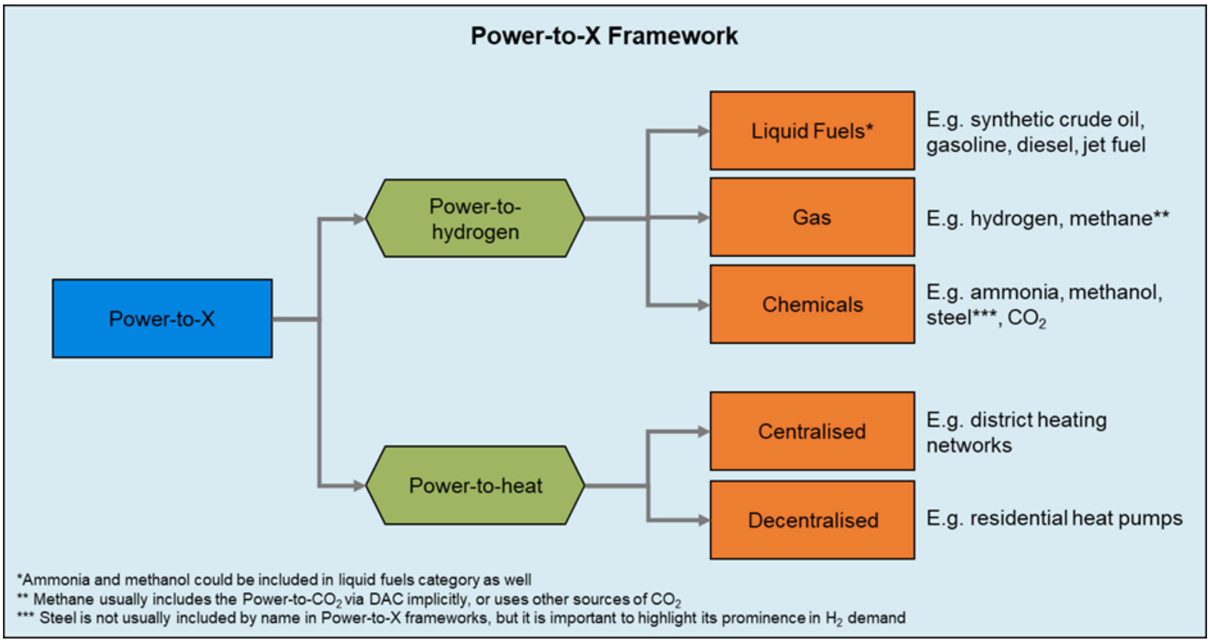


Figure 2.4: Power-to-X conceptual framework adapted from [5].

2.4.2.2 Overview of Sector Coupling in ESM

Widespread sector coupling would be a fundamental paradigm shift in the power system, as the system moves from inflexible demands met by flexible supply of power to a system of flexible demands met by inflexible VRE supply which is dependent on weather [111]. ESM are increasingly including sector coupling to various degrees in order to understand how this paradigm shift would affect our future, decarbonised grids. Findings of these models often find that sector coupling brings benefits to the wider system, like reducing curtailment, reducing system costs, lowering the costs to decarbonise hard-to-abate sectors, reducing the need for supply side flexibility such as batteries and long-duration storage, etc.[111–115].

The risks of ignoring sector coupling potential and continuing the current path of decoupled sectors is that societies will build unnecessary infrastructure, such as more flexibility than required in the electricity generation via storage. While achieving an optimal system design may prove to be impossible, the historical precedence of decoupled sectoral planning and operation will miss this valuable opportunity. Therefore, integrated, whole system analysis must become the new norm for regional and national electricity system planning. This is a daunting prospect, but nevertheless crucial for a technically, economically, and environmentally efficient decarbonised system. Moreover, this analysis cannot just be done once. Sector coupling will likely have both general outcomes which are uniform across countries as well as very specific outcomes based on a country's context of renewables, sectoral demands, etc.

Finally, it is clear that this new paradigm requires more coordinated electricity system operation and planning. There is still much progress needed in market design and regulation, business models, and ownership and governance [110]

2.4.2.3 Transport Sector coupling

Transport sector coupling has focussed almost exclusively on the potential of BEV charging to give and take electricity from the grid on a daily timescale, i.e., "smart" charging or Vehicle to Grid (V2G) [116]. Pilot projects are being implemented in Europe [117, 118]. Many ESM consider V2G interactions for reducing daily storage needs [113, 115, 119–121].

He et al. [122] also consider the sector coupling of hydrogen for transport, in this case in an ESM-based analysis of the northeast USA grid. He et al. [122] considered a flat weekly hydrogen demand for transport in light- and heavy-duty Fuel Cell Electric Vehicles (FCEV), omitting other key sectors such as chemicals, steel, and aviation and shipping fuels. Like BEV, the demand for hydrogen is flat over any duration longer than a day, and thus the sector coupling potential is limited to intra-daily effects on the power system design and operation. Aboveground hydrogen storage proves to be too expensive in the model to store beyond a daily level.

2.4.2.4 Thermal Sector coupling

In addition to the transport sector, many ESM include thermal sector coupling in ESM [111–113, 115, 120, 121]. For example, Zhang et. al [112] model residential and industrial heating with an electricity planning and dispatch model to 2030 for Great Britain. Similar to other ESM results, Zhang et al. find that sector coupling of heat with the electricity sector reduces overall system costs by 3-8% compared to a decoupled system by reducing the need for flexibility assets in the electricity sector [112].

Both cooling and heating offer significant load shifting on a daily level [110], while longer duration demand is effectively an additional fixed constraint on the system (either flat in industrial use cases such as refrigeration, or seasonal in residential use cases with the outside temperatures). This intra-daily flexibility can reduce the need for short duration storage. The seasonal demand profile can either facilitate or impede VRE integration, depending on the seasonal shape of the relevant VRE profiles. Importantly, this seasonal demand shape is not within the control of the energy planners or electricity system operators, but rather a function of outside temperature. Thus, it does not provide seasonal *flexibility* for managing the system.

While the ESM investigation into transport and thermal sector coupling is quite advanced for daily flexibility, in the case of **seasonal** load shifting, which is the focus of this thesis, the electric vehicle transport and thermal sectors are not really relevant for a sector coupling investigation. There is little opportunity for load shifting potential on timescales longer than a day in these two examples of sector coupling, while chemical sector coupling does offer this potential.

2.4.2.5 Chemical Sector coupling

Chemical sector coupling potential includes power-to-hydrogen and subsequent products (e.g., synthetic hydrocarbons, ammonia, steel) for chemicals, transport, and re-electrification. Chemical sector coupling also includes flexible chemical production (e.g., aluminium electrolysis, papermaking, cement, chlorine, etc.). In the system, chemical sector coupling has numerous potential benefits, including addressing hard to abate sectors, reducing fossil fuel imports via substitution with local PtX, providing long duration storage (power-to-X-to-power) or reducing the need for long duration storage (seasonal production), ancillary services via fast response electrolysers, and reducing stranded assets.

There have been several analyses of the sector coupling potential in the EU which include chemical sector coupling. Here, three streams of sector coupling research are reviewed which include the chemical sector coupling potential in some capacity. Notably, chemical sector coupling using Balmorel as an ESM is intentionally excluded from this review because it is reviewed in the subsequent section.

First, in an ESM-based study of 80% decarbonising in the EU by 2050, the EU ASSET project (De Vita et al. [115]) showed early indications of the use of sector coupling for providing seasonal storage in underground hydrogen storage infrastructure and in pipelines. While pointing towards the usefulness of seasonal flexibility, the implications do not go far enough due to limiting techno-economic and decarbonisation assumptions. For example, De Vita et al. use hydrogen storage for industrial users, such as ammonia fertiliser production, but consider these demands to be flat instead of allowing production to vary. The only storage considered is underground storage, either of hydrogen or of synthetic methane. Any storage in another form (e.g., ammonia storage tanks, piles of steel) are not considered. Furthermore, significant hydrogen and ammonia demands are omitted, such as aviation and shipping transport fuel, which is either not decarbonised (80% decarbonisation scenario rather than net-zero) or is met by biofuels [115].

Secondly, PyPSA, an open sourced ESM capable of sector coupling, has been used in numerous studies to investigate the role of sector coupling in a European context [113, 120, 121]. Brown et al. [113] investigate transmission and sector coupling of heat and transport in the European context and find significant benefits to the system costs. Power-to-methane is included; however, the study only covers 72% of European energy demand, with non-electric industrial demand (17%), shipping (5%) and aviation (4%) excluded [113], and thus overlooks the major role of chemical sector coupling. Similar findings are found in Victoria et al. [120], who look at the role of storage technologies in sector coupled European system using PyPSA, but again, the analysis omits the sectors of industry, shipping, aviation and agriculture. The most recent iteration of this model found in Victoria, Zeyen, & Brown [121] includes the sectors of shipping and aviation; however, there are other limitations which prevent a deep investigation of the potential of chemical sector coupling. First, shipping is assumed to use hydrogen, even though ammonia or synthetic liquid fuels are considered the path towards shipping decarbonisation. This matters because these fuels can be stored much cheaper than hydrogen, and therefore have more potential for seasonal production load shifting. Secondly, hydrogen demand for steel and ammonia fertiliser production is considered to be flat. Thus, any flexibility in these industrial users, as well as shipping, can only come in the form of underground hydrogen salt cavern storage [121]. These two limitations prevent the full seasonal sector coupling potential from being included in the modelling.

Thirdly, Gils et al. [123] consider the role of sector coupling to a very detailed level in a net-zero Germany energy system by 2050. They utilise sector coupling potential in transport, heat, and chemicals via hydrogen and methanation. The findings point towards an important role in seasonal hydrogen production and storage in salt caverns by 2050 at a level of 53 TWh, as well as seasonal methanation and storage [123]. Unfortunately, neither flexible ammonia production nor ammonia storage are included in the study. This omission is quite common across the literature on ESM which Gils et al. [124] review in a literature review on sector coupling representation across models. The only inclusion of hydrogen flexibility found in the literature review is when hydrogen electrolysis is paired with salt cavern storage and/or methanation and underground methane storage [124]. Furthermore, Gils et al. [123] do not include shipping or aviation fuel.

Beyond these three branches of leading research in sector coupled ESMs, other ESM studies in the European context have focused on sector coupling of synthetic methane production, which is then used in various existing gas infrastructure, including heating, industry, and power [113, 114]. The challenges with synthetic methane include the costs compared to alternatives in these sectors, while the advantages include the ability to utilise existing gas infrastructure, such as gas turbines, gas boilers, and the gas grid. Additionally, uncertainty surrounds methane emissions from leakage and the source (and costs) of CO_2 for production of synthetic methane. Nevertheless, synthetic methane has garnered far more attention than ammonia to date in the chemical sector coupling space.

There are other sector couplings as well, with aluminium, steel, cement, chloride and paper production having flexibility potentials to operate at loads as low as 25% of maximum load [110], which could provide seasonal load shifting in the form of stockpiles of aluminium, steel, cement etc. or with international trading with inverse production schedules in other regions. This concept appears to be unexplored to date and could be researched as future work resulting from the findings of this thesis.

In summary, the chemical sector is included in several sector coupled ESM of the European energy system, but there are several research gaps. No study includes any chemical storage besides underground hydrogen and methane storage. Also, no study considers flexible chemical processes, such as flexible ammonia synthesis, flexible shipping fuel production, or flexible steel production. Finally, many studies exclude industrial, aviation, and shipping demands.

2.4.3 Sector coupling in Balmorel and Optiflow

Three examples of recent work in Balmorel investigate the potential for sector coupling.

First, Ikäheimo et al. [80] use Balmorel to model green ammonia for fertiliser and dispatchable power generation in Northern Europe to 2050. The study finds significant ammonia is used to transport electricity from Norway to Germany, to be used for fertiliser and to be combusted for re-electrification. However, Ikäheimo et al. do not consider flexible Haber-Bosch Synthesis Process (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.

Secondly, Lester et al. [125] use an OptiFlow add-on coupled with Balmorel to model the sector coupled electricity, heat, and transport sector in the Nordic and German region in 2050. This study highlights the role of biomass in providing fuels for transport, especially aviation and shipping, as well as the role of district heating demand being met by waste heat from other industries (synthetic fuel production for aviation and shipping, municipal waste burning, data centre waste heat). The main limitation of this model, from the perspective of this thesis, are that is does not consider any storage besides aboveground hydrogen and CO_2 storage (i.e., no ammonia storage or synthetic fuel storage) nor does it consider flexible ammonia or synthetic fuel synthesis. These assumptions prevent any seasonal load shifting of ammonia or synthetic fuel production from being considered. Additionally, other chemical sector demands are overlooked, such as steel, fertiliser, etc. Nevertheless, the methodology of the OptiFlow add-on for investigating sector coupling provided a basis for this thesis's work.

Thirdly, Gea-Bermúdez et al. [111] use a Balmorel-based model to consider sector coupling of heat, EVs, as well as synthetic fuels for aviation and shipping in Northern-central Europe. Like previously reviewed sector coupling studies, the findings highlight far less battery storage required due to heat and EV sector coupling. Additionally, the results showcase the usefulness of transmission and sector coupling together, but also highlight scenarios where public acceptance limits further transmission lines. Interestingly, the production of synthetic fuels for aviation, shipping, and hydrogen for hydrogen FCEV transport are considered to be somewhat flexible, with a peak-to-average demand ratio of electricity consumption of 1.5, i.e., the plants must average a capacity factor of 67% throughout the year [111]. Unfortunately, this is a constraint dictated by the authors without much justification, rather than a constraint limited by the processes' inherent flexibilities or an economic optimum.

A major weakness of this model is that it only considers hydrogen storage in aboveground tanks, which is very expensive. This also causes a logical gap in the system; the results depict a seasonal pattern of production of synthetic fuels using the limited flexibility, yet the demand is likely relatively flat, and no synthetic fuel storage is included in the model [111]. The annual demand of synthetic fuel is met, but it is not met on a weekly level. Indeed, the authors highlight a limitation in the modelling of the synthetic fuels demand, which should be modelled with the appropriate technologies (e.g. production, storage, transport, end-use, and potential conversion back to power) rather than just an electricity demand with arbitrary flexibility [111]. Nevertheless, the limited flexibility in the synthetic fuel production for aviation and shipping is a significant first step in the research to date, and the results clearly point towards the usefulness of this flexibility in the system.

Beyond seasonal load-shifting of synthetic fuels, another result from Gea-Bermúdez et al. foreshadows the results presented in Chapter 5 of this thesis. Gea-Bermúdez et al. included the technology option for synthetic methane, using CO_2 from DAC, and injected it into the grid (without storage) for use in power generation, heat, and combined heat and power plants. They find that this technology is *only* deployed, mostly in combined heat and power plants, in scenarios where sector coupling of the transport sector (including shipping and aviation fuels) is *excluded* from the model run. In other words, the flexible production of synthetic fuels appears to reduce the need for X-to-power re-electrification technologies.

2.5 Electricity System Modelling in India

The ESM-based studies of India have predominantly focused on the integration of high levels of wind and solar into the grid in the near-term. More recently, studies have included the electrification of transport, industry, and buildings, and started to explore the role of hydrogen. The relevant ESM-based studies of India of the last several years are listed in Table 2.2 along with their focus, key strengths, and weaknesses from the perspective of this thesis. In general, these reports use capacity expansion and generation dispatch ESMs of the Indian electricity grid to 2030 (except [68, 126] to 2040 and [127, 128] to 2050).

Most of the reports are focused on the near-term requirements to VRE integration, such as thermal power plant (i.e., existing coal and gas plant) flexibility requirements and battery storage required for new solar and wind power by 2030. Indeed, the IEA reported, "India has a higher requirement for flexibility in its power system operation than almost any other country in the world" [68]. Surprisingly, sector coupling approaches which are commonly used in European focused ESMs, like time-shifting BEV and thermal demands to reduce battery storage requirements, are completely overlooked. Focusing on interim systems of roughly 20% to 40% decarbonised electricity systems is undoubtedly important for keeping the lights on amidst rapid VRE deployment in India, but likely misses path dependent decisions and policies which will steer the system towards a better final state. Hopefully, the recent announcement of net-zero by 2070 by the Indian government at COP26 [66] will prompt more long-term, deep decarbonisation modelling in the big institutions leading the Indian ESM research, such as National Renewable Energy Laboratory (NREL) [127, 129, 130], Lawrence Berkeley National Laboratory (LBNL) [131], The Energy and Resources Institute (TERI) [2, 132], Niti Aayog [133], and International Energy Agency (IEA) [68, 133].

The limited amount of sector coupling which has been included has focused on the potential for shifting agricultural irrigation pumping to day-time hours to better use the solar electricity which is available on the grid [131, 133]. Agricultural load shifting is seen as the lowest hanging fruit for shifting some 60 GW of agricultural load to solar hours, and already has been successful in shifting 6 GW in 2020 in several states (e.g., Karnataka, Maharashtra, and Gujarat) [131]. However, this is the limited extent of the focus of any demand side response in the modelling of India to date.

Title	Year	Author	Notes
Greening the Grid [129]	2017	NREL	• First major work to address Indian electricity system decarbonisation. • Focus is meeting Paris climate conference ambition of new solar and wind by 2022 • Strengths include aggregating essential data on demand and supply for all future ESM. • Gaps include a very limited time horizon and thus no focus on transformational effects of VRE integration, such as sector coupling.
India 2030 Wind and Solar Integration Study: Interim Report [130]	2019	NREL	• Focus on meeting Indian government's 2030 targets for VRE deployment of 40% renewable electricity capacity (including hydropower) by 2030 • Strengths include spatially and temporally granular dispatch model, and specifically investigating the role of transmission expansion. • Weaknesses include exogenous capacity expansion (i.e., not optimally chosen by the model, but defined by user inputs), no sector coupling or demand side flexibility considered, one year of weather data.
Renewable Power Pathways: Modelling the Integration of Wind and Solar in India by 2030 [132]	2019	TERI	• Focus on updated Indian government target of integrating 450 GW of VRE by 2030 • Strengths include spatially and temporally granular dispatch model, and specifically investigating the usefulness of coal power plant flexibility alongside batteries. • Weaknesses include exogenous capacity expansion (i.e., not optimally chosen by the model, but defined by user inputs), no sector coupling or demand side flexibility considered, one year of weather data.
Report on Optimal Generation Capacity Mix for 2029-30 [134]	2020	CEA	• Central Electricity Authority (CEA) is the Government's electricity system planning body • Focus is the planned capacity expansion to 2030, especially short duration storage in batteries and pumped hydro. • Strengths include clear government assumptions on hydro expansion, batteries and VRE. • Weaknesses include no mention of hydrogen or ammonia or sector coupling.
The Potential Role of Hydrogen in India [2]	2020	TERI	• Focus is the role of hydrogen in India to 2050. • Strengths include strong industrial sector analysis for decarbonisation and hydrogen demand (including ammonia for fertiliser). • Weaknesses include not including hydrogen / ammonia demand for shipping and aviation, nor any role of sector coupling of hydrogen. Report suggests for hydrogen production to be islanded from the grid (opposite findings of this thesis) to minimise hydrogen costs, while not considering sector coupling benefits for the system.
The Role of Transmission Grid and Solar Wind Complementarity in Mitigating the Monsoon Effect in a Fully Sustainable Electricity System for India [128]	2020	Gulagi et al.	• Focus is a 100% decarbonised Indian grid by 2050 • Strengths include the use of chemical storage (synthetic methane) for seasonal balancing of the system, and a relatively ambitious investigation into net-zero by 2050. • Weaknesses include no sector coupling potential, only using one year of weather data, and only considering synthetic gas (no ammonia).
India's potential for integrating solar and on- and offshore wind power into its energy system [126]	2020	Lu et al.	• Focus is 80% decarbonisation of Indian electricity system by 2040. • Strengths include a relatively ambitious investigation into 80% system decarbonisation by 2040 compared to the other literature. • Weaknesses are many. These include (i) very pessimistic solar cost reduction potential, and thus a wind dominated outcome (outlier in the literature), (ii) only battery storage considered, (iii) no sector coupling or hydrogen / ammonia included, (iv) only one timestep considered, no pathways,
India Energy Outlook 2021 [68]	2021	IEA	• Focus on Indian energy system, including electricity, transport, industry, cooking fuel, etc. • Strengths are many – this is 250 page report. Notable strengths include aggregation of historical, current, and future projections of demand and emissions across sectors, putting Indian aspects into global contexts. • Weaknesses include pessimistic cost reductions, no sector coupling even though hydrogen for industry is considered in some scenarios, a focus on natural gas infrastructure and import expansion in India. Also assumes islanded hydrogen is the cheapest, citing on TERI's H2 report.
Renewables Integration in India [133]	2021	IEA & Niti Aayog	• Focus is integration of VRE to 2030, especially in states with highest VRE penetration, using batteries and pumped storage, some demand side flexibility, thermal power plant flexibility, and transmission. • Strengths include country wide and Gujarat state hourly dispatch models (considering operating costs, plant technical minimum operating levels, minimum up and down times, start-up times and ramp rates), sector coupling of agricultural irrigation pumping, policy deep dive. • Weaknesses include no hydrogen or industrial sector coupling, pessimistic cost reductions, not a capacity expansion model (exogenously determined capacity)
Energy Storage in South Asia: Understanding the Role of Grid-Connected Energy Storage in South Asia's Power Sector Transformation [127]	2021	NREL	• Focus is quantifying role of battery and pumped hydro storage to 2050 • Strengths include modelling of capacity market payments and operating reserve requirements. • Weaknesses include: (i) no sector coupling considered, (ii), no CCS, hydrogen, or ammonia considered, (iii) using weather data from 2014, (iv) cost declines assumed 1.1%/yr decline for solar, 0.82%/yr decline for onshore wind
Least-Cost Pathway for India's Power System Investments through 2030 [131]	2021	LBNL	• Focus is flexible resources such as energy storage, load shifting, gas, and electricity markets to 2030 • Strengths include sector coupling of agricultural irrigation pumping for load shifting • Weaknesses include no sector coupling outside of agricultural loads, no hydrogen or ammonia considered.

Table 2.2: Literature review of ESM-based studies of the Indian electricity system.

2.5.1 Gaps in Indian ESMs

Four common gaps are highlighted in the literature of ESM in India: i) not considering hydrogen and ammonia sector coupling, ii) using unrealistically pessimistic cost reduction forecasts of key components, iii) using one year of weather data, and iv) only modelling to 2030, and thus limited VRE penetration.

First, the role of industrial demand side response using electrolysers is not considered in any of the studies. Hydrogen is increasingly being studied for the Indian electricity system, prompted by the government's National Hydrogen Mission (NHM) [67] and TERI's seminal report highlighting the massive scale of the green hydrogen and ammonia industries [2]. While TERI's report is a major contribution to the literature, and indeed used as a basis for many of the data input assumptions of this thesis, the report does not use a system-wide optimisation model to investigate the role of sector coupling of hydrogen and ammonia. In just looking at the hydrogen sector alone, TERI recommends that hydrogen production proceed in an islanded configuration, decoupled from the electricity grid to avoid grid connection charges which stymie industry connection in India today [2]. This narrow view of the system misses the huge sector coupling potential in significantly reducing system costs. Foreshadowing the results of this thesis, TERI finds that in a decoupled system, significant hydrogen is needed for long-duration electricity storage (i.e., power-to-hydrogen-to-power), amounting to up to 10% of final electricity in a net-zero grid [2].

Secondly, most of the models have unrealistically pessimistic cost reductions of RE technology. Almost all of the reviewed models use expert estimate based cost projections for the key components, which, as described in Chapter 4, has been proven to be systematically biased in the case of VRE technologies [135]. This is especially prominent in the IEA models as shown in Figure 4.2. Lu et al. [126] is a particularly illustrative case of erroneous input cost assumptions leading to undesirable results. Lu et al. forecast Indian solar capital costs to be 550 to 1650 USD kW^{-1} by 2040, while the actual cost as of 2020 reported by IRENA was 596 USD kW^{-1} and still rapidly dropping [136]. Unsurprisingly, Lu et al. design an Indian electricity system which is dominated by onshore wind, rather than solar PV, which is markedly different than all long-term models reviewed of the Indian system. One model, NREL [127], approaches cost declines in a somewhat learning-based manner. They assume cost declines of 1.1% per year decline for solar and 0.82% per year decline for onshore wind which gradually reduces to 0% by 2050. This methodology could be seen as a modified version of Moore's law, but still lacks the empirical rigour of Way et al. [137] to justify these cost declines, or indeed to include the backdrop of a global decarbonisation-based deployment scenario.

Thirdly, most of the models are not adequately spatially resolved for RE profiles, and none of the models consider more than one year of weather data. This is a significant weakness for India, which has a large interannual variation in wind resource (as shown in Chapter 4). Given that many of the studies are focusing on short duration storage and thermal plant ramping requirements in the near-term, it is surprising that they continue to use one year of typical weather data which will underestimate the storage requirements. NREL [127] potentially mitigates this limitation by including operational reserves at 5% of national demand in each time slice, and a planning reserve margin of 15% of peak demand in each region. Nevertheless this reserve margin strategy is not validated using multiple year of weather data or a statistical based analysis for the system, and thus is completely arbitrary.

Fourthly, most of the models only extend to 2030, and thus less than 50% VRE penetration. This limited planning prioritises short-term costs at the cost of a potentially more optimal long-term system. Additionally, this limited decarbonisation can ignore other sectors, such as industry, aviation, and shipping; however, these sectors realistically need to start decarbonising in this decade because of the long lifetime assets, and thus should be included in modelling today. Moreover, the government of India has made clear policy targets in the recent weeks [18] which target huge green hydrogen and ammonia deployment before 2030, and thus need to be included in power sector modelling.

2.6 Motivation for the research

Despite such clear signals towards the significant role of green ammonia in net-zero societies and the wave of investment into green ammonia production plants, the integrated, sector coupled role of power-to-ammonia, ammonia storage and transport, and ammonia-to-power, have not been sufficiently explored or quantified in the literature. Foremost, there are gaps in foundational models of power-to-ammonia and ammonia-to-power which this thesis seeks to fill. These models are needed as the building blocks of more advanced modelling. Secondly, analyses published using ESMs, the dominant tool for understanding different scenarios of decarbonisation, have systematically overlooked the dynamic integration of sector coupling of green ammonia (and green hydrogen, in large part) for industrial demands, such as steel and fertiliser, and for heavy-duty transport fuel in net-zero decarbonised energy systems.

The main focus in the ESM sector coupling literature to date is on short-duration, intra-daily load shifting, such as coordinated charging of Battery Electric Vehicle (BEV) fleets [116, 119], flexible heating and cooling demands [112, 138], and agricultural irrigation pumping [131]. Several analyses of parts of the European energy system are beginning to investigate sector coupling of hydrogen for various sectors, such as aviation and shipping fuel, industry, and heating [111, 121, 123]. 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 models to date 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.

As previously highlighted, India is an ideal case study due to clear policy signals towards large-scale domestic green hydrogen and ammonia production [18, 67], a non-marginal electricity demand for electrolysers compared to the grid (Figure 1.4), and seasonal storage needs due to the monsoon weather pattern. Despite the scale of the required electrolyser fleet, there is not a modelling effort that considers the dynamic role of industrial electrification and 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 [68, 126, 127, 129–134]. Many of these ESM analyse the development of new generation, transmission, and storage assets, as well as the best way to utilise existing assets. However, all studies to date are overlooking the massive role of green hydrogen and ammonia sector coupling on facilitating the integration of high levels of VRE, reducing the cost of decarbonisation, and reducing the need for long-duration storage.

3 | Foundational Models: LCOA and ammonia-LCOE

3.1 Introduction

Ultimately, to answer the research question around the role of green ammonia in decarbonised electricity systems, a highly spatially and temporally granular ESM of an electricity grid with novel ammonia and hydrogen sector coupling is needed. This ESM is detailed in Chapters 4 and 5; however, several sub-models and higher level analysis are first needed as building blocks for this complex ESM. These building block models are developed and the results presented in this chapter.

These models also provide a first pass answer to sub-question 1: “Should green ammonia be used for re-electrification in power grids?” via an LCOE analysis. LCOE is the foremost metric for measuring an electricity generation technology’s economic competitiveness. To compare green ammonia at this benchmark level required the development of novel chemical process modelling and techno-economic modelling of both the production of ammonia and the generation of electricity from ammonia, which are described in this chapter. LCOE analysis allows for a direct comparison between technologies given specific input assumptions. Since green ammonia fuel cost is a required input to the LCOE analysis of ammonia-to-power, the output of the LCOA model of this chapter is directly linked as an input to the LCOE analysis.

The overall objective of this chapter is to provide the foundational modelling of power-to-ammonia-to-power which can be used for providing data input into more advanced energy systems models in Chapters 4 and 5, as well as provide initial results on sub-research question 1.

The specific objectives of this chapter are: (i) to forecast green ammonia LCOA from solar PV and explore its sensitivities, and (ii) to forecast a green ammonia-to-power LCOE in the electricity sector, and to compare it with alternatives, e.g., CCS and nuclear power, in order to highlight scenarios where green ammonia may be competitive in the electricity sector in the future.

This chapter is segmented into three main sections: (i) LCOA modelling, including novel methodology and results of this methodology, (ii) ammonia-to-power LCOE modelling, including novel methodology and results of this methodology compared with other dispatchable electricity generation technologies, and (iii) conclusions drawn from this stand-alone power-to-ammonia-to-power LCOE analysis. This chapter is largely based on the published research article *Ammonia to power: Forecasting the levelized cost of electricity from green ammonia in large-scale power plants* (Applied Energy 2021) [74].

3.2 Modelling LCOA

A key input to LCOE analysis of ammonia-to-power is the cost of the ammonia "fuel." Therefore, the first step towards modelling ammonia-to-power on an LCOE basis, and thus answering research sub-question 1, is to model power-to-ammonia, i.e., LCOA. As highlighted in the literature review of LCOA modelling, there are two identified gaps in LCOA modelling: first, there is no simple methodology which builds a plant that is functional and accurately represents LCOA, and secondly there are no LCOA models which consider grid connecting ammonia plants which are integrated into a larger electricity grid which is changing over time. The gap of grid connected LCOA analysis will be addressed in the following chapters, while this section focuses on the gap of a simple, yet accurate LCOA model.

In answering research sub-question 1 and comparing the LCOE of ammonia-to-power with alternative technologies, a location independent model is desired. One approach to generating this input cost of ammonia could have been to use a global average of literature values from published complex modelling approaches, such as [6, 72, 77]. However, there are problems with using these models to come up with a general ammonia "fuel"input price. Salmon et al. [72] is not a global model, and focuses only on Australia in 2020. Nayak-Luke [6] provides costs at over 500 global locations, but only extends to 2030, and does not include battery technology, which is found to be crucial for creating cheaper ammonia in optimised models of both [72] and [77]. Fasihi et al. [77] is global to 2050 and includes batteries, but is pessimistic on electrolyser cost declines, and thus green ammonia LCOA declines are limited.

Therefore, there was justification for exploring a simple methodology for LCOA which was global and generic in nature, customised to this research's assumptions, and validated with the complex models. A simplified techno-economic model, called Generic Solar Ammonia Model (GSAM), was developed in Microsoft Excel to fill this gap and to provide LCOA as an output, which would be used as the ammonia fuel cost input assumptions to the ammonia-to-power LCOE model. The LCOA has been calculated for 2020–2040 to determine the realistic fuel cost of green ammonia and to highlight key sensitivities. For GSAM, the key inputs are techno-economic assumptions including cost forecasts over time, as well as plant design and operational philosophy which dictate key process equipment sizing. The key outputs of GSAM are LCOA over time and a sensitivity analysis.

3.2.1 Methodology: Generic Solar Ammonia Model

To forecast the LCOA, the production cost of green ammonia was modelled using an industrial scale green ammonia synthesis plant, using solar PV as the energy source. The process flow diagram is shown in Figure 3.1 and the techno-economic assumptions are listed in Table A.1.

GSAM focuses on green ammonia generation via solar PV (and not wind or solar-wind hybrid plants) for three reasons. First, solar PV was found to exclusively dominate the plant designs in the global complex models from 2030 onwards in both global modelling research publications [6, 77]. Using 2020 costs, [6] finds that solar PV and wind are more competitive with one another and [77] similarly finds wind-solar-battery hybrid plants are most competitive in the near term; however, due to sharper forecasted declines in solar PV costs compared to wind, solar PV is found to dominate optimised plant design in the long term. As this ammonia-to-power model is focused on the mid to long term after 2030, solar PV based green ammonia production systems are more relevant for modelling ammonia input costs. Secondly, the diurnal variability associated with solar is easier to predict and thus it is simpler to design generic optimised plant solutions. Most notably, wind power plants can endure weeks without substantial wind resources, even in favourable wind locations. This can result in challenging plant design configurations for maintaining the HB minimum load, and a surprisingly high LCOA, given the rated capacity factor of the resource. On the other hand, solar PV power plants in favourable locations are far more steady and do not exhibit weekly periods of insufficient resource. Thirdly, favourable solar PV resources are widely available across the globe, and justify the assumption in the geographically independent LCOE analysis that ammonia will be widely available at this calculated price. The solar irradiation levels assumed for GSAM are 2,000 FLH, which can be found in the USA and Central America, South America, India, China, northern Africa, southern Africa, the Middle East, Australia, and southern Europe, i.e., on every continent [139], thus justifying the *global* applicability of the methodology.

All equipment is sized using a binary daily profile as shown in Figure 3.2, assuming that all of the required hydrogen is produced when solar electricity is available. While real solar

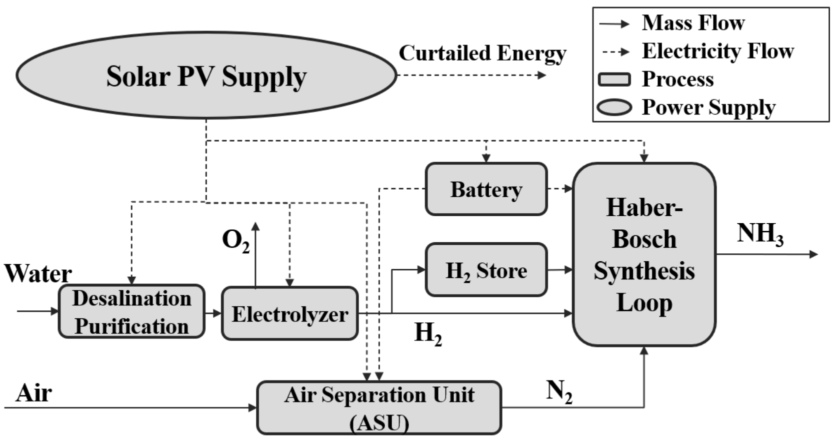


Figure 3.1: Green ammonia synthesis process flow diagram as modelled in GSAM

PV profiles are not binary, solar PV with tracking is closer to this binary profile as the tracking specifically improves the energy received at the morning and late afternoon. The binary assumption is a simplification that may limit the relevance to more equatorial locations without seasonal effects to hours on sunlight per day. However, the binary plant design also assumes inherent conservative elements that may enable the plant to operate in many conditions. The conservative elements include that the HB synthesis loop is running at full load during the entire day, which creates conservative oversizing of the electrolyser and hydrogen storage to maintain the hydrogen consumption. In reality, the plant could turn down to maintain hydrogen reservoirs at night and on cloudy days.

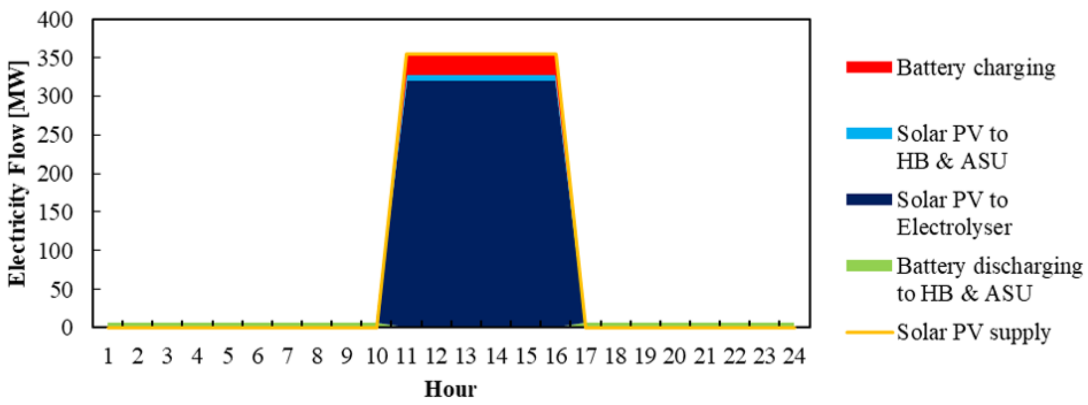


Figure 3.2: Power allocation for 10 t NH_3/hr green ammonia synthesis plant using GSAM methodology for plant equipment sizing

In the GSAM process, hydrogen is stored in above ground hydrogen tanks at 200 bar to allow for a constant supply of hydrogen to the HB synthesis loop. The electricity requirement of the HB and ASU is powered by battery storage when solar electricity is not available, and thus the batteries are also conservatively sized. The binary profile assumption is a large simplification which allows for simple plant sizing, is shown to match well with more complex models. GSAM was validated against the complex model in [6] in locations which produce green ammonia from solar PV, as shown in Figure 3.3. When considering locations with only solar PV, GSAM shows an LCOA error of less than 10%, given the same input assumptions. The comparison suggests that GSAM is capable of modelling a very similar LCOA to complex models for solar-only locations.

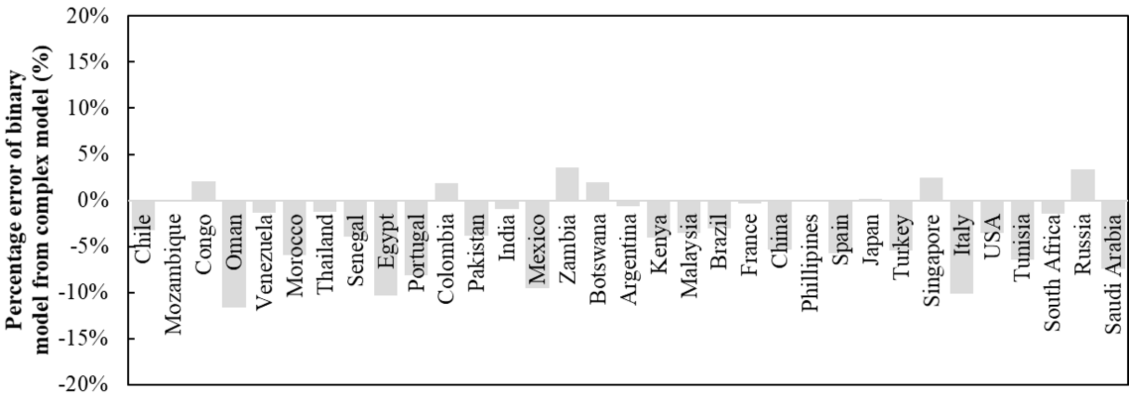


Figure 3.3: LCOA percentage error between simplified GSAM LCOA methodology (i.e. "binary model") and methodology used in [6] at 33 locations using solar PV with single axis tracking

In islanded green ammonia production systems, some form of electricity storage is needed, either via hydrogen consumed in hydrogen fuel cells or hydrogen GTs, or via batteries, to maintain the electricity demands of the compressors in the ASU and HB when VRE is not available. Nayak-Luke [6] utilises hydrogen fuel cells, but does not consider batteries as a technology option. Both Salmon et al. [72] and Fasihi et al. [77] include batteries as a technology option and find that batteries, especially when paired with solar PV based systems, are the least cost form of back-up power when compared to hydrogen fuel cells and gas turbines. Therefore, this analysis assumed batteries provide the back-up power for the HB and ASU when there is no power coming from the solar PV. As further validation of the plant design, a large-scale green ammonia plant announced in Neom, Saudi Arabia, appears to have a similar process flow to Figure 3.1 [140]. The sizing of the equipment of Neom has not been confirmed, but there are batteries included as part of the design, validating the useof batteries for back-up power in GSAM.

The LCOA was calculated using equation 3.1

$$LCOA = \frac{\sum_{t=0}^{n} \frac{C_t + O\&M_t}{(1+r)^t}}{\sum_{t=0}^{n} \frac{A_t}{(1+r)^t}} \tag{3.1}$$

where:

$C_t =$ Investment expenditures in year t

$A_t =$ Ammonia produced in year t

$O\&M_t =$ Operations and maintenance expenditures in the year t

$n =$ economic lifetime of the plant

$r =$ Weighted average cost of capital (WACC)

The LCOA cost breakdown in 2040 is shown in Figure 3.4. The solar PV resource used in the GSAM considers solar PV with single axis tracking because it is becoming the standard, with over 70% of the solar PV installed annually in the USA today being solar PV with single axis tracking [141].

The storage of electricity and hydrogen are key cost components of the plant, and make up 12% of LCOA costs in 2040, as shown in Figure 3.4. Notably, the batteries are not providing electricity storage for the hydrogen production via the electrolyser, but rather the electrolyser is

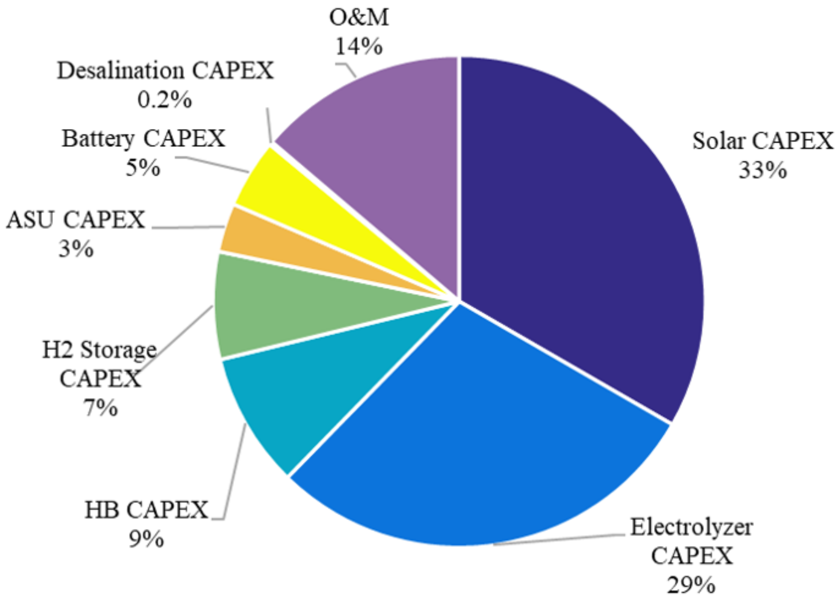
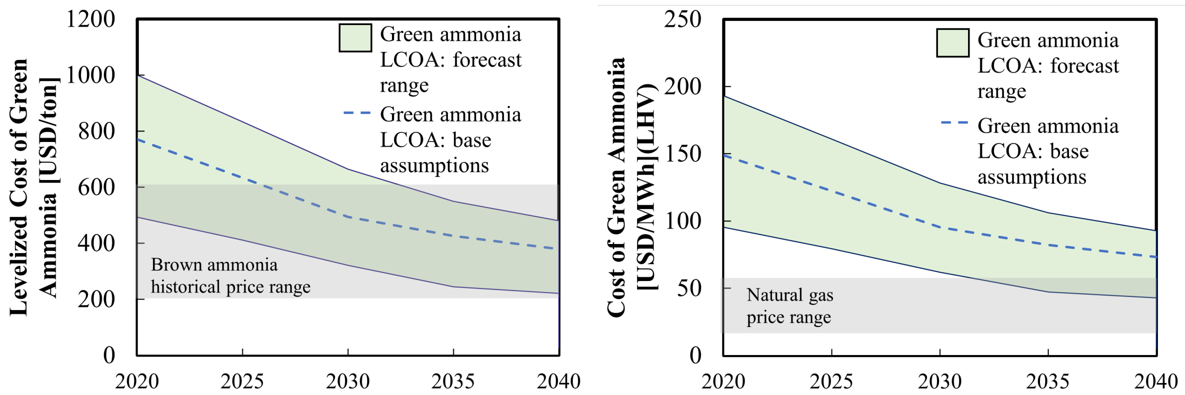


Figure 3.4: LCOA cost breakdown for 2040 using GSAM, base assumptions listed in Table A.1

operating on a diurnal schedule with the solar resource. The batteries are only used for the less electricity intensive HB and ASU processes, as shown in Figure 3.2. In short, stored electricity is assumed to be simply too expensive to use to generate hydrogen.

One weakness of the GSAM is the hydrogen storage buffer, which is assumed to require one to two days of storage in above-ground tanks at 200 bar. It is not a modelled quantity, but rather a user input assumption. This limitation is why GSAM is only used to model solar-based ammonia plants, as wind droughts require a more complex methodology for optimising hydrogen storage volume. One to two days of storage is therefore conservative in the GSAM case, as it is impossible to have zero solar PV for one to two days: even in cloudy situations, considerable power is generated. The estimate of two days in 2020 is reduced to one day on 2040, based on similar assumptions from hourly plant process level simulation from [76] using sites in South America. The key parameter for reducing onsite hydrogen storage requirements even further is increased HB flexiblity. No real plants have been built to validate claims around HB flexiblity, and thus GSAM assumes constant HB operation. However, plants at the 10 - 100



(a) LCOA results of GSAM (b) LCOA on MWh/t basis, compared with NG

Figure 3.5: a. Green ammonia production cost forecasted 2020 to 2040 with historical fossil fuel based ammonia price range of 200–600 USD/t [7]. LCOA range calculated using low and high literature estimates for electrolyser CAPEX, WACC, and solar PV LCOE (simultaneously), as presented in Table 3.1)(note: FLH sensitivity is not included), b. LCOA compared on USD / MWh (LHV) basis, comparison with natural gas 5-15 USD/MMBTU (HHV)

Metric Tonne per Day (MTPD) scale have been announced in Denmark [37], Scotland [36], and Australia [41] to explore higher HB flexibility designs.

3.2.2 Results of GSAM: LCOA forecasts to 2040

The results of GSAM for a solar location with 2,000 FLH is shown in Figure 3.5a. The results suggest that green ammonia may be competitive with historical brown ammonia prices almost immediately, and certainly very competitive by 2040. The comparison of this LCOA on an energy basis is shown in Figure 3.5b, with recent historical natural gas prices of 5 - 15 USD/MMBTU shown for comparison. Notably, these natural gas prices do not consider any CO_2 taxes, and yet still the results suggest that an achievable LCOA may begin to compete with natural gas in the 2030s. Figure 3.5b sets the scene for the core research questions of this research in examining the role of ammonia in the electricity sector as a carbon-free, dispatchable chemical fuel replacement for natural gas.

Sensitivity analysis

The sensitivity analysis conducted with GSAM highlights the vast uncertainty that affects LCOA predictions. As shown in Figure 3.5a, the range of LCOA values is very large, even in present day predictions, and this range is maintained over time. The range of LCOA shown in Figure 3.5a is calculated using low and high literature estimates for electrolyser CAPEX, WACC, and solar PV LCOE (simultaneously), as presented in Table 3.1 (note: FLH sensitivity is not included). One paramount reason for this uncertainty is the uncertainty in electrolyser prices, both in present day as well as in the future. The other key sensitivities, as highlighted in Figure 3.6, are the Weighted Average Cost of Capital (WACC) and the renewables LCOE and FLH. The sensitivity analysis was conducted by changing one variable at a time, and thus the results are non-additive. The baseline LCOA for 2040 is 380 USD/t, as shown in Figure 3.5a, using data from Table 3.1. The average low and high LCOA from the sensitivity estimates for 2040 is 294 USD/t and 450 USD/t, respectively.

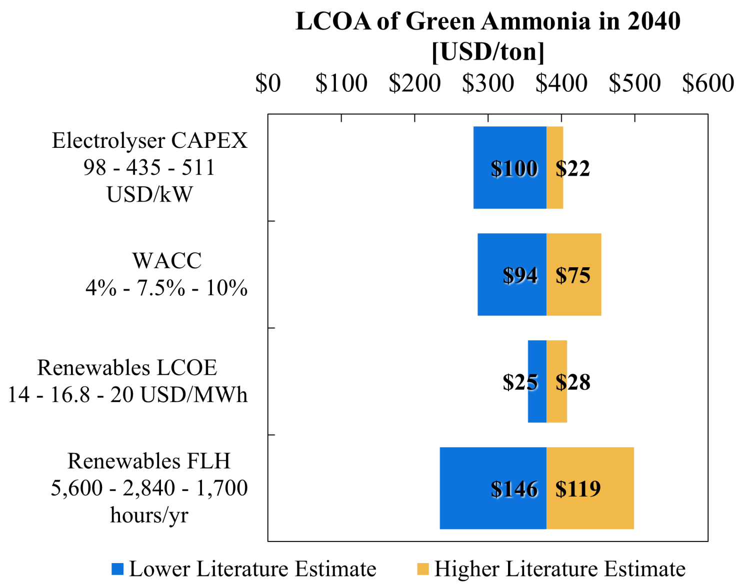


Figure 3.6: GSAM LCOA key sensitivities in 2040 based on low and high values from the literature, see Table 3.1

Current electrolyser Capital Expenditure (CAPEX) estimates range from 200 USD/kW for large scale alkaline electrolysis in China (400 USD/kW outside of China) [142] to Interna-

	2020	2025	2030	2035	2040	Unit	Reference
Electrolyser CAPEX							
Lower literature estimate	400	264	115	106	98	USD / kW	Bloomberg NEF[142]
Base estimate	770	655	540	488	435	USD / kW	IRENA 2020 [143]
Higher literature estimate	939	834	730	600	511	USD / kW	Upper estimate from IEA[24] and [144]
Weighted Average Cost of Capital (WACC)							
Lower literature estimate	4.0%	4.0%	4.0%	4.0%	4.0%	%	Offshore wind in Europe has achieved 4% in 2018[145]
Base estimate	7.5%	7.5%	7.5%	7.5%	7.5%	%	Standard used in IRENA analyses for OECD and China[146]
Higher literature estimate	10.0%	10.0%	10.0%	10.0%	10.0%	%	Developing country assumption in IRENA analyses[146]
Solar PV LCOE (widely achievable)							
Lower literature estimate	24	22	20	15	14	USD / MWh	IRENA Solar PV low of 20 USD / MWh in 2030 and 14 USD / MWh in 2050 [143].
Base estimate	29	24	19	18	17	USD / MWh	See Appendix Table A.1. Calculated from component costs and widely achievable solar irradiation.
Higher literature estimate	34	28	23	21	20	USD / MWh	Assuming IRENA Solar PV low forecast for 2030 [143] is not achieved until 2050.
LCOA from Solar PV							
Lower estimate	493	412	321	244	222	USD/t NH_3	See Appendix Table A.1 for further methodology
Base estimate	771	634	494	426	380	USD/t NH_3	See Appendix Table A.1 for further methodology
Higher estimate	1,000	834	664	550	480	USD/t NH_3	See Appendix Table A.1 for further methodology
Renewable Full Load Hours*							
Lower literature estimate	1,500	1,500	1,500	1,500	1,500	hr/yr	IEA average capacity factor of 23% for USA PV in 2040 [145]
Base estimate	2,000	2,000	2,000	2,000	2,000	hr/yr	See Appendix Table A.1.
Higher literature estimate	5,600	5,600	5,600	5,600	5,600	hr/yr	64% wind/solar combined capacity factor available in Patagonia [76]

*RE FLH sensitivity not used to calculate LCOA range in 3.5a due to overlapping effects with solar PV LCOE. Single variable sensitivity presented in 3.6

Table 3.1: LCOA Sensitivity assumptions

tional Renewable Energy Agency (IRENA) global estimates of 770 USD/kW [143], to upper estimates of over 900 USD/kW by the International Energy Agency (IEA) [24]. This uncertainty in prices is in part due to few real-world recent data points at over 10 MW scale. This is likely to be resolved in the next years as large-scale electrolyser projects are built. The prospects for an electrolyser boom are evident in post-COVID recovery packages, with 6.5, 5, 4, and 2 GW announced targets by 2030 in France, Germany, Spain, and Portugal, respectively

[147]. Pre-COVID, at the end of 2019, the installed global capacity of electrolysers was 250 MW [148] and the pipeline of projects to 2030 was only 3.5 GW [149]. The long-term IRENA forecasts for 1,700 GW by 2050 [150] seems far more achievable with the dramatic ramping up of announced projects.

The results of the sensitivity analysis also highlight the potential for lower financing costs (i.e., WACC) to significantly reduce LCOA as well as the effect of regional differences in RE resources, as captured by the variables of RE FLH and LCOE in Figure 3.6. Fundamentally, a green ammonia plant including the solar PV is almost entirely CAPEX, so the sensitivity to WACC is unsurprising. Notably, the combination of low WACC, e.g. 4% which matches UK offshore wind [145], and low electrolyser costs in 2040 of 90 USD/kW [142], would result in LCOA of circa 200 USD/t.

The LCOE uncertainty range for solar PV is relatively small, from 14 USD / MWh to 20 USD / MWh, because the forecasts for solar PV LCOE are all quite consistent. Unsurprisingly, there is little effect on the LCOA with such small forecast variation.

Finally, the high sensitivity to RE FLH highlights two important considerations. First, the higher FLH of 5,600 hours per year highlights the potential for wind plants and wind/solar hybrid plants to affect LCOA significantly. However, an important caveat is that the LCOE would likely increase with wind (which is not shown in the single variable sensitivity analysis) and the plant requirement for hydrogen storage may be significantly higher given the risks of long periods of wind droughts. Secondly, the case of only 1,700 FLH highlights the advantage of sunnier locations and using solar PV with single axis tracking, which increases the FLH from 2,000 to 2,840 hours per year in the base case.

In conclusion, the GSAM provides a foundation of the range of achievable LCOA over time, using widely available solar PV resources with single axis tracking and a plant design as outlined in Figure 3.1. A single variable sensitivity analysis was conducted to highlight the potential for green ammonia to be a competitive fertiliser feedstock before 2030, and fuel by 2040, given favourable techno-economic developments. The modelling used in the more advanced models of Chapter 5 have notable improvements on GSAM, specifically grid connected green ammonia instead of islanded, both solar and wind based designs, granular hourly VRE profiles over many years instead of a generic 24 hour profile, and learning-curve-based cost assumptions instead of expert estimates. Despite these meaningful improvements, the techno-economic modelling of GSAM is useful to create transparent and relatively accurate LCOA estimates which justify further research into green ammonia as an energy vector. Indeed, GSAM prefaced the expected LCOA which would be later found in the detailed India case study (Chapter 6).

3.3 Modelling LCOE of Ammonia-to-power

After modelling LCOA, the second step towards modelling power-to-ammonia-to-power on a stand-alone LCOE basis is to model ammonia-to-power. Again, this LCOE model is useful as a first pass at answering research sub question 1: "Should green ammonia be used for re-electrification in power grids? How does using green ammonia for dispatchable power generation compare with traditionally modelled low-carbon technologies for dispatchable power, such as fossil fuel with CCS, nuclear energy, and bioenergy with or without CCS?"

The literature review in Chapter 2 highlighted a gap in the literature around techno-economic comparison of green ammonia-to-power at power plant scale, with no example in the literature to date. Furthermore, within this modelling of ammmonia-to-power, there is a gap in modelling the comparison between various integrated cracking scenarios, i.e., whether the gas turbine is fuelled by pure ammonia, fully cracked to hydrogen, or a partially cracked mix. This section aims to fill these gaps.

As inputs to this LCOE model, the techno-economic parameters are needed for an ammonia-to-power system, as well as the relevant fuel, O&M, and CAPEX costs. For the ammonia-to-power system, key values are fuel efficiency and CAPEX. To model these for different plausible ammonia-to-power scenarios, chemical engineering modelling of the integrated cracking and power plant was required.

3.3.1 Methodology: Ammonia Gas Turbine Model

An ammonia-to-power CCGT system was selected for lowest possible LCOE at power plant scale (100s of MW) based on cost and high Technology Readiness Level (TRL) technology. Ammonia-fueled CCGT systems can combust hydrogen derived from ammonia [9], or a blend of ammonia and hydrogen [151], or ammonia directly. This analysis groups ammonia combustion technologies as pure hydrogen (Phase 1), blends of hydrogen and ammonia (Phase 2), and pure ammonia (Phase 3), in line with current industry research and development, and progress towards lower LCOE. The configurations analysed in this thesis are presented in Figure 3.7.

Ammonia cracking techno-economic analysis

Forecasting the LCOE of Phases 1 and 2 requires a chemical process model and a techno-economic analysis of an integrated ammonia decomposition system with CCGT.

The heat required for the high temperature thermocatalytic reforming of ammonia into hydrogen can be generated by cannibalising a fraction of the decomposed product stream and burning this hydrogen rich stream in a fired reformer (i.e., a cracker). This approach is similar

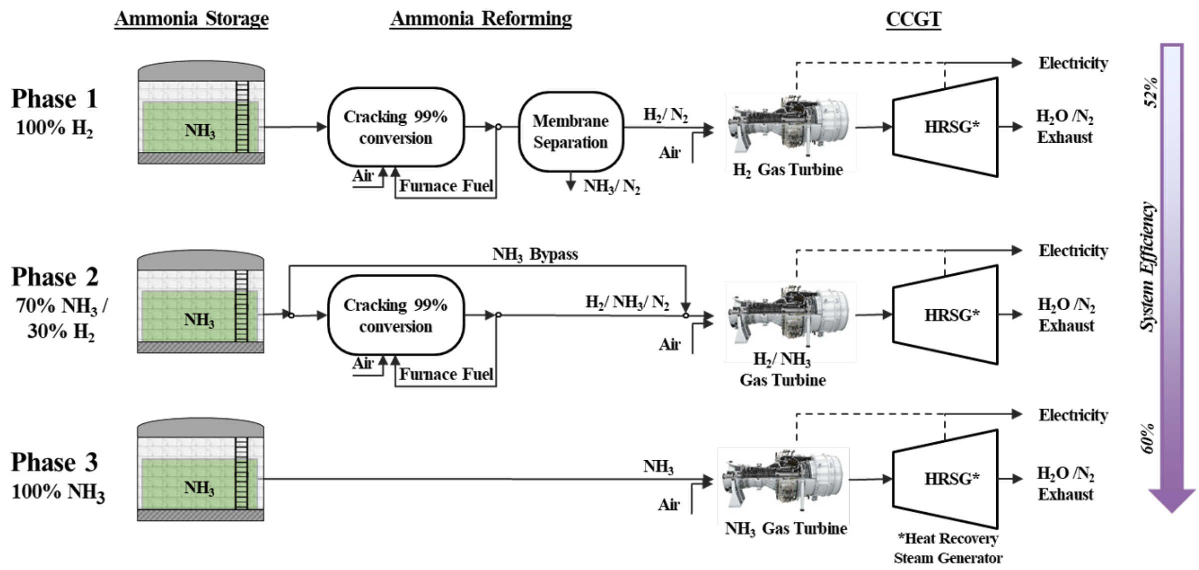


Figure 3.7: Ammonia fuelled CCGT configurations as modelled in three cases of 100% H_2, 70% NH_3 / 30% H_2, and 100% NH_3

to the one reported in [152] and is depicted as Phase 1 in Figure 3.7. In a fully heat-integrated process, liquid NH_3 would be vaporised and preheated using the low-grade heat of the exhaust stream. The integrated system in Phases 1 and 2 were modelled in ASPEN Plus (see Figure 3.8 and Table 3.2) to determine the heat integration, required rate of cannibalisation, and overall system ammonia-to-power efficiency. The system CCGT was based on Siemens SGT-800, a medium (62.5 MW) turbine already capable of running on 50% H_2 [153]. In the modelled reformer, 99% conversion was assumed at 850 °C. This conversion and temperature assumption was based on small-scale commercial ammonia decomposition reactors, which use nickel catalysts at 850 °C [154, 155]. Literature suggests high conversion cracking is achievable between 650 °C and 900 °C depending on the catalyst [156]; however, for low cost and high technological maturity, nickel catalyst has been found to be the most cost-effective catalyst [157].

The technology for ammonia cracking is commercially available at small scale (i.e., less than 100 kg H_2/hr output) [154, 155, 158]. Large scale cracking can be modelled using SMR as a basis, due to the analogous thermocatalytic cracking reactor design employed. Large-

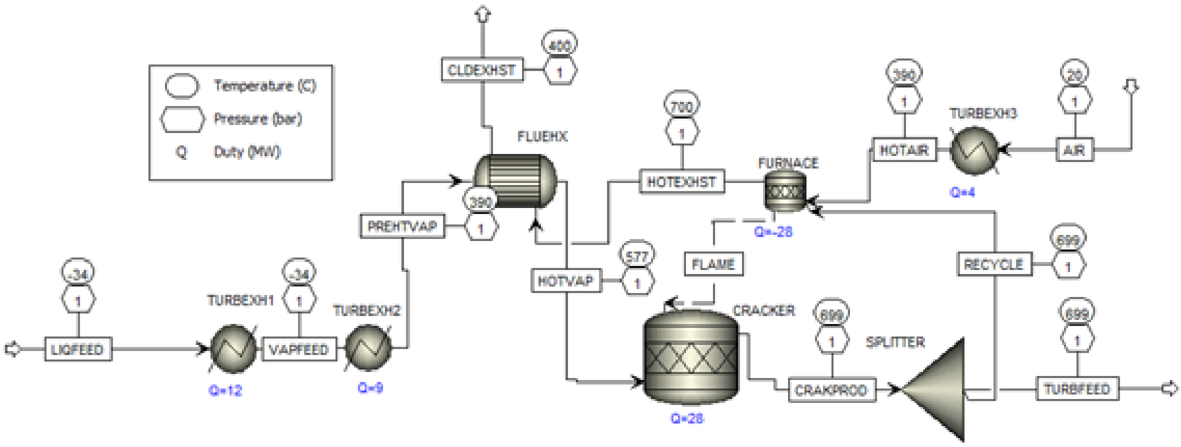


Figure 3.8: ASPEN Plus v9 model of an ammonia decomposition reactor system with waste heat recovery from CCGT system (turbine exhaust is TURBEXH1, 2, 3)

scale, thermocatalytic reformers for SMR are large fireboxes with dimensions at the scale of a building [159], with significant impact of economies of scale on cost reduction. In a large scale cracker, ammonia would be fed through parallel, vertical, catalyst filled tubes, which are arranged in the firebox [160]. The design would closely resemble SMR because both processes are constrained by maintaining high enough reaction temperature inside the tubes against the endothermic cracking reaction (ΔH = 31 kJ/mol H_2 in NH_3 decomposition versus a slightly higher SMR ΔH = 41–69 kJ/mol H_2). This design constraint is managed through the design of the tube diameter and firebox temperature. Based on analogous designs, literature values of actual SMR installed CAPEX costs as well as several ammonia cracker installed CAPEX estimates are plotted in Figure 3.9, and a power regression is fit to the installed CAPEX curve.

In Phase 1, the cannibalisation stream was calculated to be 20.5% of the product stream using an ASPEN model of the system shown in Figure 3.8 with specifications outlined in Table 3.2. Due to this fuel cannibalisation in the pre-treatment cracking stage, overall fuel efficiency (based on the LHV of ammonia) was thus reduced to 52.5% from the base 60% CCGT efficiency. Phase 2 has a fuel efficiency of 57.4%, using a scaled model of Phase 1, with most of the ammonia bypassing the efficiency losses in the cracking stage. For Phase 3, the baseline

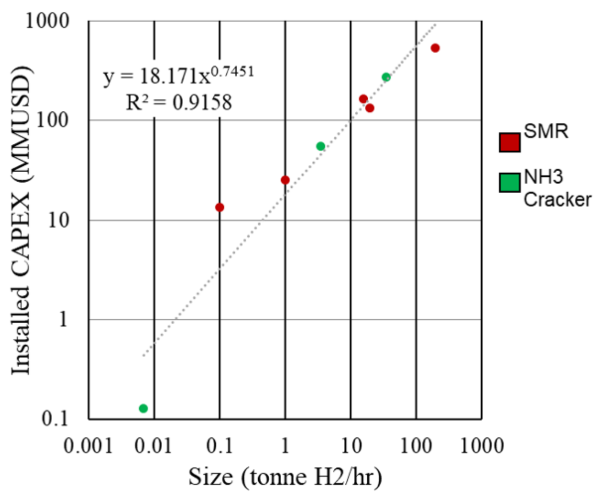


Figure 3.9: Cracker cost curve: Ammonia Reformer Installed CAPEX cost curve based on literature values for ammonia crackers at 0.007 [8], 3.6 and 36 ton H_2/hr [9] and SMR at 0.10, 1.0, 20, 200 ton H_2/hr [10], and SMR at 15.8 ton H_2/hr [11]

CCGT fuel efficiency is expected to be around 60%.

The ammonia reformer was the only additional CAPEX considered for an ammonia CCGT system compared to a natural gas CCGT system. Costs for ammonia storage tanks were disregarded in this analysis because they were assumed to be the same cost as for LNG. Due to the overlapping properties, some storage tanks for LNG can even be used for the storage of ammonia [59].

3.3.2 Ammonia-to-power LCOE results versus alternatives

The LCOE can be broken down into component costs for fuel, installed CAPEX, O&M, and emissions. Techno-economic input assumptions for supercritical pulverised coal power plants with CCS, natural gas CCGT with CCS, nuclear, Bio-energy with Carbon Capture and Storage (BECCS), and the three phases of ammonia CCGT shown in Figure 3.7 are summarised in Appendix Table A.2. The LCOE for each Phase was calculated using Equation 3.2 [162].

Key user defined variables		**Unit**	**Reference**
TURBFEED Flow Rate	4.4	tH_2/hr	Calculated based on Siemens SGT800 82 MW CCGT 1 x 1 configuration, 60% fuel efficiency, assuming same fuel efficiency for H_2 as natural gas [161]
CRACKER reactor conversion	0.99	%	Based on cracking achieved in small-scale commercial ammonia decomposition reactors [155] [154]
CRACKER outlet temperature	700	C	Literature suggests high conversion cracking is achievable between 650 °C and 900 °C depending on the catalyst [156]
LIQFEED temperature	-34	C	
Excess air ratio	1.12		
Process Units			
TURBEXH1, TURBEXH2, TURBEXH3	Heat exchangers modelled as heaters. Assuming heat from turbine exhaust is 400 C and Delta T is 10 C.		
FLUEHX	Heat exchanger. Delta T min = 10 C.		
CRACKER	Fired ammonia decomposition reactor modelled as 2 x RGIBBS reactors. CRACKER is ammonia decomposition reaction.		
FURNACE	Fired ammonia decomposition reactor modelled as 2 x RGIBBS reactors. FURNACE is hydrogen and trace ammonia combustion reaction		
SPLITTER	Separator to recycle some of ammonia decomposition reactor products to fire the furnace.		
Required Convergence			
SPLITTER	Recycle stream size converged to satisfy ammonia decomposition reactor constraints		
LIQFEED	Liquid ammonia feed mass flow rate converged to satisfy constraints of system output to gas turbine		
Results			
SPLITTER recycle %	20.5%		

Table 3.2: ASPEN Plus v9 modelling assumptions and results

$$LCOE = \frac{\sum_{t=0}^{n} \frac{C_t + O\&M_t}{(1+r)^t}}{\sum_{t=0}^{n} \frac{E_t}{(1+r)^t}} \tag{3.2}$$

where:

C_t = Investment expenditures in year t

E_t = Electricity produced in year t

$O\&M_t$ = Operations and maintenance expenditures in the year t

n = economic lifetime of the plant

r = Weighted average cost of capital (WACC)

The resulting average LCOE for each of the Phases for green ammonia-to-electricity are shown in Figure 3.10. Compared to other prominent low-carbon options, green ammonia is most competitive at low power plant capacity factors, specifically below 25%, which is shown in Figure 3.11. While capacity factors above 50% are common today for dispatchable electricity generation [145], projections into the future suggest much lower capacity factors. For example, the IEA identified capacity factors as low as 15% for peaking gas turbines in future energy systems [24], and Bloomberg New Energy Finance (BNEF) identified 25% as an approximate capacity factor required for dispatchable generation in scenarios compatible with 2 °C decarbonisation [12].

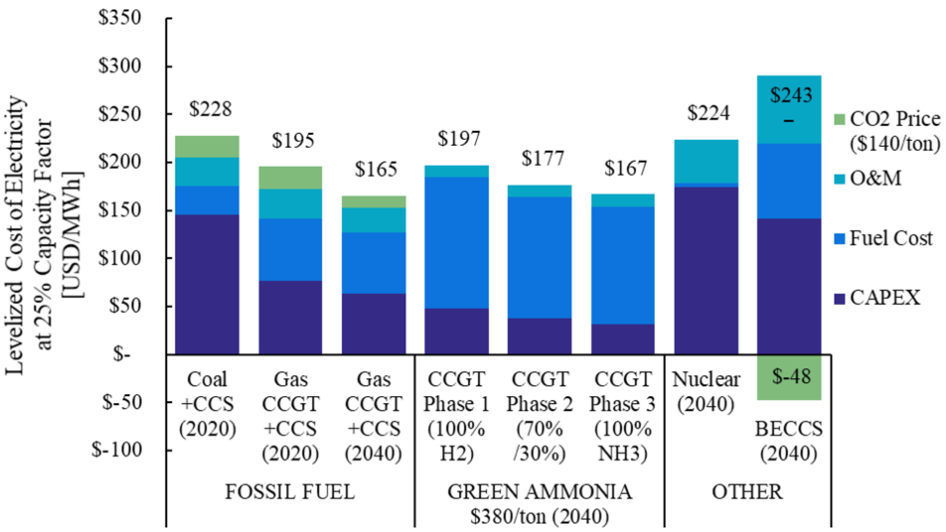


Figure 3.10: LCOE comparison of low/no carbon dispatchable electricity using EU electricity sector assumptions at 25% power plant capacity factor based on BNEF capacity factor forecasts in high VRE penetration scenarios [12]

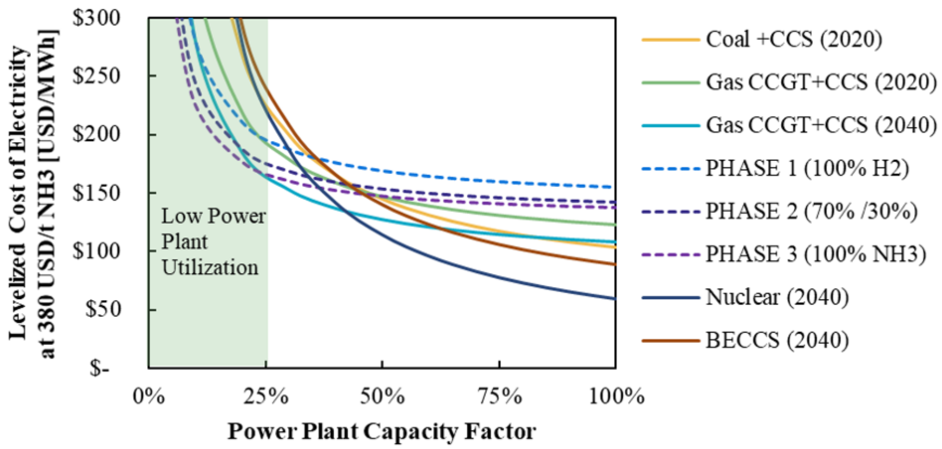


Figure 3.11: LCOE of low/no carbon dispatchable electricity at a range of power plant capacity factors

Based on the assumptions listed in Appendix Table A.2, ammonia direct firing in CCGT (i.e., Phase 3 technology) has an LCOE of 167 USD / MWh at a 25% power plant capacity factor, with the only marginally lower LCOE generated in gas CCGT with CCS using future cost assumptions (30% reduced in CAPEX and OPEX from 2020 to 2040 [163]).

However, the uncertainties surrounding these LCOE figures are high. The key sensitivities considered for green ammonia's LCOE are the fuel price, the WACC, the power plant capacity factor, and the NH_3 firing compatibility (i.e., Phase 1, 2, or 3 ammonia CCGT technology). Table 3.3 highlights low and high estimates for key model inputs in 2040, as found in the literature, and Figure 3.12 shows the LCOE sensitivity. The LCOE is most sensitive to the fuel price estimates and power plant capacity factor. Green ammonia fuel price, i.e., LCOA, is subject to wide uncertainty, with more potential on the lower end, as shown in Figure 3.6.

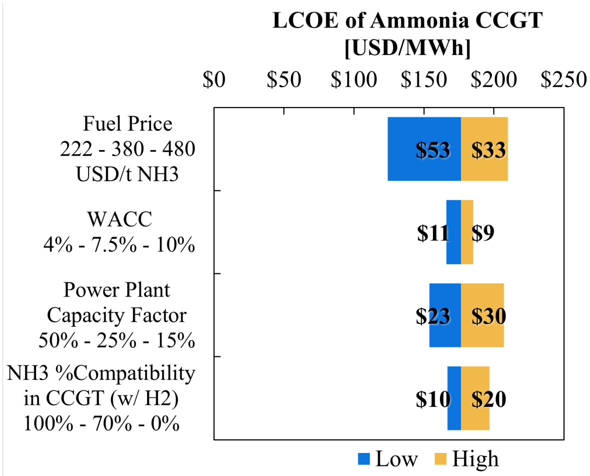


Figure 3.12: Sensitivity analysis of LCOE in 2040 based on low and high values for key model inputs

Figures 3.10, 3.11 and 3.12 highlight the cost differences in the three phases of ammonia CCGT technology (i.e., NH_3 compatibility). Phases 2 and 3 have 10% and 15% lower LCOE than Phase 1, respectively. These results highlight the value for CCGT manufacturers to pursue pure ammonia combustion. As mentioned previously, this result was corroborated by industry in the recent announcement of Mitsubishi targeting pure ammonia combustion by 2025 in a 40 MW turbine [60].

Comparing with CCS

	2040 Forecast	Unit	Reference
Fuel Price			
Lower literature estimate	222	USD/t NH_3	Based on lower estimates in electrolyser CAPEX, WACC, and solar PV LCOE (see Table 3.1)
Base estimate	380	USD/t NH_3	Base estimates, as shown in Appendix Table A.1
Higher literature estimate	480	USD/t NH_3	Based on higher estimates in electrolyser CAPEX, WACC, and solar PV LCOE (see Table 3.1)
Weighted Average Cost of Capital (WACC)			
Lower literature estimate	4	%	Offshore wind in Europe has achieved 4% in 2018 [145]
Base estimate	7.5	%	Standard used in IRENA analyses for OECD and China [146]
Higher literature estimate	10	%	Developing country assumption in IRENA analyses [146]
Power Plant Capacity Factor			
Lower literature estimate	0.15	%	Lower capacity factor used by [24] for H_2 peaking gas turbines in future energy systems
Base estimate	0.25	%	Identified as approximate capacity factor for technology required for 2C decarbonisation in [12]
Higher literature estimate	0.5	%	Gas CCGT capacity factor forecasted for USA, China, and India in [145] in 2040
NH_3 %Compatibility in CCGT (w/ H_2)			
Lower literature estimate	0	%NH_3 by volume	Phase 1 (see section 3.3.1)
Base estimate	0.7	%NH_3 by volume	Phase 2 (see section 3.3.1)
Higher literature estimate	1	%NH_3 by volume	Phase 3 (see section 3.3.1)

Table 3.3: Ammonia CCGT LCOE Sensitivity assumptions

CCS is the dominant low-carbon, dispatchable technology used in energy systems models, with over 400 GW of fossil fuel with CCS deployed by 2050 in the IEA forecasts [145]. However, the results of this analysis suggest that green ammonia firing in CCGT may achieve lower costs by 2040, or at least will be very competitive, and therefore should be included in prominent models.

In addition to fossil fuel combustion with CCS, BECCS is a widely discussed concept for achieving net negative CO_2 emissions. The results suggest that ammonia to power is over 20% lower cost at low plant capacity factors. Furthermore, there is uncertainty in the negative emissions provided based on land-use change, fuel transport costs, and the energy required to grow biomass [164, 165]. There are also uncertainties in the biomass available for BECCS [165] as well as other sectors looking to use biogenic sources, such as aviation fuel.

Green ammonia enjoys several important advantages over CCS-based alternatives beyond LCOE. Firstly, green ammonia is geographically independent with low transport costs and high likelihood to be available in all ports if it becomes widely used in the shipping sector. CCS requires nearby underground storage or expensive CO_2 transport to suitable underground storage locations. For example, in geologies such as India's, CO_2 storage locations are widely distributed and small, causing CCS transport and storage to be very expensive [2]. Secondly, ammonia CCGT or even RICE can easily scale down to tens of MW, providing useful balancing services to a more decentralised grid of the future. Both nuclear and CCS, on the other hand, are often considered at only GW scales [145]. Thirdly, CCS and nuclear plants have limited ramp rates and cannot be frequently turned off, while ammonia could also be used in open cycle GT configuration or in RICE, which offers high dispatch flexibility [166]. Fourthly, upfront capital costs for ammonia CCGT are substantially lower. Ammonia CCGT electricity production is dominated by fuel costs, while CCS-based electricity is dominated by CAPEX, as shown in Figure 3.10. Per kW installed, ammonia CCGT adds 402 USD/kW in Phase 1, while CCS adds 1,116 USD/kW for gas CCGT and 1,426 USD/kW for supercritical coal (Appendix Table A.2). The first commercial CCS projects are forecasted to cost around 1 billion USD and take more than five years to design and build [145]. The smaller scale potential of ammonia CCGT favours more projects, sooner, and thus higher potential for cost reductions from experience curves. Finally, CCS technologies are at best 90–95% effective at capturing emissions [163], while ammonia CCGT is fundamentally carbon-free.

3.3.3 Limitations to LCOE model

The LCOE model is a first-of-a-kind, but does include significant assumptions in an uncertain space, as highlighted in the sensitivity analysis. The scenario of phases 1, 2 and 3 attempt to capture some of the uncertainty, but there are still notable limitations.

It is important to highlight the risk of NOx emissions from ammonia combustion. Fossil fuel combustion produces NOx emissions because of nitrogen in the surrounding air in the combustion chamber and the high temperatures of combustion reacting nitrogen and oxygen in the chamber to form NOx. In the case of ammonia combustion, nitrogen is present in the combustion chamber both in the air and from the fuel. The complete combustion reaction of ammonia produces N_2 (nitrogen gas) and H_2O (water), however NOx and N_2O side products do occur in reality today in ammonia combustion [151].

The proposed methods for mitigating NOx emissions from ammonia combustion are two-fold. First, there are ongoing efforts to redesign the combustion to reduce or eliminate NOx formation (e.g., a rich-lean style combustion in a gas turbine shows promise [151]). Combustion R&D is ongoing in academia and industry to reduce or eliminate NOx emissions from ammonia combustion. Secondly, post-combustion NOx removal can be achieved via the existing Selective Catalytic Reduction (SCR) process. This is the 'fail-safe' approach, which will add some cost to the combustion of ammonia. SCR is currently used to de-NOx flue gas at coal plants and in diesel engines (e.g., AdBlue in diesel cars). Interestingly, SCR uses ammonia (or urea which quicky decomposes into ammonia) sprayed over a catalyst to reduce the NOx to N_2 and H_2O.

For coal plants which have relatively high NOx emissions, the CAPEX of the SCR is usually an additional 100 to 200 USD/kW [167]. Compared to the base 2,328 USD/kW installed CAPEX for coal plants assumed in this research (see Table A.2), the SCR represents roughly 5 to 10% of installed CAPEX of the coal plant. However, the CAPEX of installed gas CCGT plants is far smaller, at 766 USD/kW, and therefore the SCR may impact the LCOE considerably, depending on the level of NOx which needs to be cleaned up. Additionally, the NOx reagent would be ammonia, which in practice might consist of combusting 99% of the ammonia fuel and redirecting 1% to clean up the flue gas; however, this percentage split will depend on how much NOx is formed, subject to the relative success of the first mitigation pathway of re-designing combustion. In summary, NOx emissions from ammonia combustion are a problem which can be overcome using existing technologies and made more economically mitigated via improved combustion R&D. At this stage, the level of NOx emissions are unknown in the public literature, and thus the costs of the SCR and ammonia fuel cannibalisation cannot be estimated. Future work should consider these costs when more data becomes available.

3.4 Conclusions from LCOE analysis

This analysis finds that green ammonia is a technically viable and economically competitive fuel for decarbonisation of the electricity sector via high efficiency gas turbine power plants by 2040. The LCOE from green ammonia is forecasted to be 167–197 USD/MWh at 25% power plant capacity factor in 2040, assuming a widely available green ammonia fuel price of 380 USD/t. This cost of electricity is comparable with natural gas power plants with post-combustion CCS and is significantly lower than coal with CCS, BECCS, and nuclear power. The additional costs of 30 USD/MWh associated with cracking ammonia to fuel hydrogen fired gas turbines suggests that gas turbine manufacturers should prioritise achieving a more ammonia compatible turbine technology in the medium to long term.

As shown in the results of the GSAM, there are large uncertainties in the production cost of green ammonia, primarily due to a wide range of forecasts of electrolyser capital cost. This uncertainty should be reduced substantially in the coming years as more large–scale electrolyser projects are deployed. A similar sized uncertainty is present in the cost of capital, which may depend on economic and political factors.

While the LCOE is a useful indicator of economic competitiveness, it is only when it is integrated into a national grid that the true economic competitiveness of green ammonia can be understood. In particular, specific grids require different capacity utilisation rates of dispatchable energy sources [105] and have different available fuel prices, including differences between domestic and imported green ammonia. Further analysis, outlined in the subsequent chapter, is required to understand the implications of such considerations at a grid or regional scale. Additional regional-specific considerations that might need to be addressed include whether a mismatch exists between low cost renewable supply and electricity demand (such as in Japan), seasonality of renewable supply, the price of competing technologies (such as the low price of gas in the USA which favours CCS technologies or hydrogen salt cavern potential in the UK), the need for flexibility (as CCGT offers less flexibility than open cycle GT), and, finally, policy decisions towards decarbonisation and supporting different technological trajectories.

In conclusion, the power-to-ammonia-to-power stand-alone LCOE analysis conducted in this thesis found clear advantages over other currently favoured alternatives, such as nuclear and CCS, which justifies integration into a national scale grid system and a deeper level of study.

4 | Advanced Models: Integrating green ammonia into an electricity system model

4.1 Introduction

Based on the findings in Chapter 2 Literature Review, it is clear that green ammonia warrants a deeper analysis in the energy sector. In the ESM research literature, gaps include that no study includes any chemical storage besides underground hydrogen and methane storage (i.e., no ammonia storage is included), no study properly considers flexible chemical processes, such as flexible ammonia synthesis, flexible shipping fuel production, or flexible steel production, and, finally, many studies exclude industrial, aviation, and shipping demands completely. The model developed in this chapter addresses all of these gaps. Furthermore, there are several gaps highlighted in the literature of ESM in India, namely not considering hydrogen and ammonia sector coupling, using unrealistically pessimistic cost reduction forecasts of key components, using one year of weather data, and only modelling to 2030, and thus limited VRE penetration. These India ESM specific gaps are also filled using the methodology outlined in this chapter.

This chapter specifically sets up the model which can answer research sub question 1: "Should green ammonia be used for re-electrification in power grids?" by developing a power-to-ammonia-to-power network add-on to the ESM. This functionality also allows the model to address subquestion 2: "What are the effects of “sector coupling” green ammonia production (for various non-power sector users such as maritime shipping fuel and fertiliser) with the electricity grid system? Should green ammonia production be grid connected or islanded?" Finally, the chapter’s detailed methodology for generating accurate solar and wind data for ESM input and developing a model which can consider 10 years of weather data sets up the model to address sub research question 3: "What are the effects of grid resilience on both potential roles (power-to-ammonia and ammonia-to-power), as explored via seasonal and interannual variation of solar PV and wind energy?"

Overall, the objective of this chapter is to develop and describe the ESM which is used to examine the research question on the role of green ammonia in decarbonised electricity systems, and address all three sub questions. This chapter provides the methodological basis of the case study on India in Chapter 5.

Specifically, the three objectives of this chapter are: (i) to justify the choice of base ESM, (ii) to improve this base ESM with three core improvements to create a novel, state-of-the-art ESM capable of modelling deep hydrogen and ammonia sector coupling, and (iii) to generate accurate, spatially and temporally granular, multi-year solar and wind profile data input for this ESM. This chapter is segmented into three main sections respectively: (i) choice of ESM (Balmorel and OptiFlow) used in this thesis, (ii) an overview of the three improvements to the ESM, and (iii) the methodology and validation results of generating multi-year solar and wind profile data inputs for the ESM.

4.2 Choosing an ESM for this research

The 17 criteria and methodology outlined in Ringkjob et al. [22] for selecting an ESM were employed, and Balmorel (with the OptiFlow add-on) was the chosen ESM. The requirements of this research question and sub-questions against all 17 criteria are shown in Table 4.1. Ringkjob et al. [22] generally break the process of choosing an ESM into four steps. Balmorel is the only model which fits all the requirements of this research. Table 4.1 down-selects other models from the 75 reviewed in [22] which are close to meeting all the requirements, but also highlights why they fail.

Regional capable model	Investment Optimisation	Operation Optimisation	Hydrogen / ammonia network	Time horizon	Comments
Balmorel	Yes	Yes	Yes	50 years (UD)	With Optiflow add-on, fits all requirements. Open source, but software (GAMS) is not free.
COMPETES	Yes	Yes	No	UD	No hydrogen or ammonia network
EnergyPLAN	Yes	No	Yes	1 year	1 year horizon, no operation optimisation
ESTAP-TIAM	Yes	Yes	Yes	2100	Low temporal resolution
NEMO	Yes	Yes	No	1 year	1 year horizon
PLEXOS	Yes	Yes	No	UD	No hydrogen or ammonia network
POLES	Yes	Yes	Yes	2100	Low temporal resolution
PyPSA	Yes	Yes	Yes	UD	Set up for PSAT originally, not set up for hydrogen / ammonia.
ReMIX	Yes	Yes	Yes	1 year	1 year horizon
SWITCH	Yes	Yes	No	UD	No hydrogen or ammonia network
TIMES	Yes	Yes	Yes	UD	Inflexible user interface and not open-source

Table 4.1: Other ESM down-selected from Ringkjob et al.[22] and the highlighted weakness compared to Balmorel

First, the model's software and availability should be considered. For this research, open-source models were preferred for starting from a mature model with a wide user base who would be able to easily uptake the results. Free software would be slightly preferred, but performance speed (often better in licensed software) is also very important for being able to build a model complex enough to address the research question while solving in reasonable times.

Second, the model's general logic is considered. This includes the first 3 criteria in Table 2.1, namely the purpose of the ESM, the approach, and the methodology. In the case of this research, the purpose of the model is both optimising on new investments for capacity expansion over time as well as operational optimisation to ensure the demand is met at every time step. The research question considers the future role of ammonia, so future investment planning is essential. Furthermore, this role is intertwined with the availability of VRE, and thus granular operational modelling is also important to understand sector coupling effects to manage VRE and how re-electrification of ammonia-to-power competes with other technologies like batteries.

The third step in choosing a model is to pick one that has the correct spatiotemporal resolution. In the case of this research, it was important to select a model capable of at least hourly dispatch modelling to capture the variation in solar PV and wind, and granularity to cover differences in solar and wind profiles across the Indian subcontinent. The model also needed to be easily applied to India with regional and state level granularity for capturing different demands and VRE supply. Finally, the time horizon needed to cover at least until 2050. Indeed many of the 75 models reviewed in Ringkjob et al. [22] were ruled out at the spatiotemporal decision step, as shown in Table 4.1.

Fourthly, the techno-economic considerations of the model need to be considered. The most relevant restriction for this research was that a model needed to be able to include other vectors besides electricity, namely hydrogen and ammonia. While none had been used for ammonia specifically, the functionality is clear in some while not present in others, as shown in Table 4.1.

While Balmorel was a relatively clear winner by satisfying all the requirements, the other model that comes close to the requirement and worth highlighting is PyPSA. Indeed PyPSA has developed significantly from the start of this research project and the writing of the review in

Ringkjob et al. [22] in 2018, and several recent PyPSA sector coupling papers are reviewed in the literature review section [113, 120, 121]. One advantage of PyPSA is that is uses free software, while Balmorel uses licensed software. However, Balmorel has advantages in many more years of use and was purpose built for capacity building and operation modelling, while PyPSA was purpose built for much more granular power system modelling and only has recently been expanded to include these new features.

In summary, the abridged ESM requirements for this research which were almost exclusively met by Balmorel can be summarised as follows:

1. Open-Source
2. Optimises investment and operation, can run different scenarios, rather than just simulating or scenario testing
3. Good temporal resolution (i.e. can be hourly) to capture variation in wind and solar PV
4. Able to do regional/international scope outside of Europe
5. Can include chemical fuels (hydrogen and ammonia) as well as just electricity
6. Flexible demand arrangements

4.3 Introduction to Balmorel and OptiFlow

4.3.1 Balmorel

To address this research's questions, Balmorel was chosen as a widely used, open source ESM. BALtic Model Of Regional Energy Liberalization (historical acronym, no longer relevant) (Balmorel) is a model which has been developed over the last two decades to support analyses of the energy sector with emphasis on electricity and combined heat and power systems[168]. The model is used for energy and environmental analyses of relevant economic and policy related issues as well as technical analyses of power and combined heat and power systems. The base model was first written for Baltic/Nordic countries and is now used worldwide. As a techno-economic model, it provides the functionality to conduct energy planning for the power and heat sector.

The model is written in General Algebraic Modelling System (GAMS), an algebraic modelling language and software used to solve linear, nonlinear, and mixed-integer optimisation problems. In its basic configuration, the Balmorel model linearly optimises 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 provided technical and economic assumptions and constraints.

The advantages of Balmorel include that it is scalable from regional to international power systems, very customisable, transparent, and transferable to stakeholders for further analyses. Balmorel is not only extensively used in Europe [111, 125, 169] but it also has been recently used to examine the energy transition in capacity building countries, and is the core model used in recent technical reports on the energy transition in China [170], Indonesia [171], and Vietnam [172]. Indeed, in the Economics of Energy Innovation and System Transition (EEIST) consortium, which has provided funding for this thesis, Balmorel is also used by the Energy Research Institute (ERI), to model the energy transition in China in their annual China Renewable Energy Outlook report [170].

Besides wide geographic scope, Balmorel is well suited to answer the key questions of PtX and PtXtP integration in energy systems. Balmorel is able to consider any range of available power generation technology options, such as coal, gas, wind, solar, nuclear, hydropower, batteries, biomass, etc. with country-specific cost forecasts and availability. The limitations of Balmorel, as used in this thesis, include a simplified representation of transmission (a single capacity between regions), short-sighted investment optimisation (no inter-year foresight to anticipate falling fuel prices or rising CO_2 prices), full intra-year foresight (hydro use, storages, and fuel restrictions using perfect prediction of wind and solar), and perfect competition in a market of economic rationality.

As a linear optimization system, Balmorel seeks to minimize an objective function Z subject to constraints. The simplified objective function for electricity only (no heat demand) for India is shown in Equation 4.1. The objective function minimizes the sum of electricity generation non-fuel and fuel costs, new generation investment costs, and new transmission investment costs. More complex versions of Balmorel add other terms, but this is the base objective function. One notable variation includes unit commitment, which considers the real cost and operational restrictions of turning power generation assets on and off over short periods of time, for example to meet peaking power demands. Unit commitment can be important when modelling granular operational constraints; however, it is not a trivial functionality to include. Adding unit commitment requires Mixed Integer Linear Programming (MILP) based approaches to solve, and thus dramatically increase calculation time to perform the optimisation. In this research, unit commitment was not included as it was considered unnecessary to answer the research questions and made calculation times untenable.

Detailed documentation of Balmorel can be found in [173] and [168]. The objective function is subject to constraint equations regarding i) electricity balance of supply and demand, ii) installed generation and transmission capacities, iii) energy levels in time (e.g. energy storage levels), iv) operational limits such as ramp rates and minimum operating load level, and v) other constraints such as CO_2 emissions limits or other policy limitations.

$$minZ_y = \sum_{g,t}(c^e_{g,t} \times G_{g,t}) + \sum_{f,g,t}(c^f_{g,t} \times F^f_{g,t}) + \sum_{g}((a \times c^i_g + c^{fix}_g)I_g) + \sum_{x}(a \times c^i_x \times I_x) \quad (4.1)$$

where:

Variables: Z: objective function (system costs), c: cost per unit of, G: generated units of electricity (MW), F: fuel consumed units of, a: annual capital recovery, I: investments (MW)

Subscript: y: year, g: generation technology (e.g., solar PV), t: timestep, x: transmission

Superscript: e: electricity, f: fuel, i: investment, fix: annual fixed costs

4.3.2 OptiFlow network model of PtX

OptiFlow [174] is an open-source spatio-temporal network optimisation 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 minimising cost is included inside Balmorel's cost optimisation 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 on the configuration used in [125, 169] and as shown in Figure 4.1.

OptiFlow is deterministic, i.e., there is no probabilistic element, and a model run will reliably produce the same result based on a specified set of inputs. The model is partial equilibrium, as it only considers the electricity sector and hydrogen/ammonia sectors, and the demand for these sectors are exogenously set and not changed by costs resulting from the model. On the other hand, IAMs are usually general equilibrium, and consider multiple non-energy sectors of the economy and feedback or relationships between these sectors.

OptiFlow is a useful add-on to Balmorel for modelling sector coupling, and indeed Lester et al. [125] use it for modelling sector coupling of the power, heat and transport sectors in Denmark in 2050, which is further reviewed in the next section.

4.4 Methodological improvements

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 4.1). As part of the EEIST project, funded by UK government Department for Business, Energy, and Industrial Strategy (BEIS) and Childern's Investment Fund Foundation (CIFF), the modelling used in this research aims to improve upon traditional modelling approaches under a new framework, called Risk Opportunity Analysis (ROA). Traditional modelling-based policy approaches, specifically Cost Benefit Analysis (CBA) and other equilibrium-based approaches, are often used to appraise or model policy decisions which will affect systems in a marginal, or incremental capacity [175]. However, the UK government and other national governments have recognised a need for different tools to appraise policy in the realm of transformational change, defined by HM Treasury in 2020 as: "[...] a radical permanent qualitative change in the subject being transformed, so that the subject when transformed has very different properties and behaves or operates in a different way." [176].

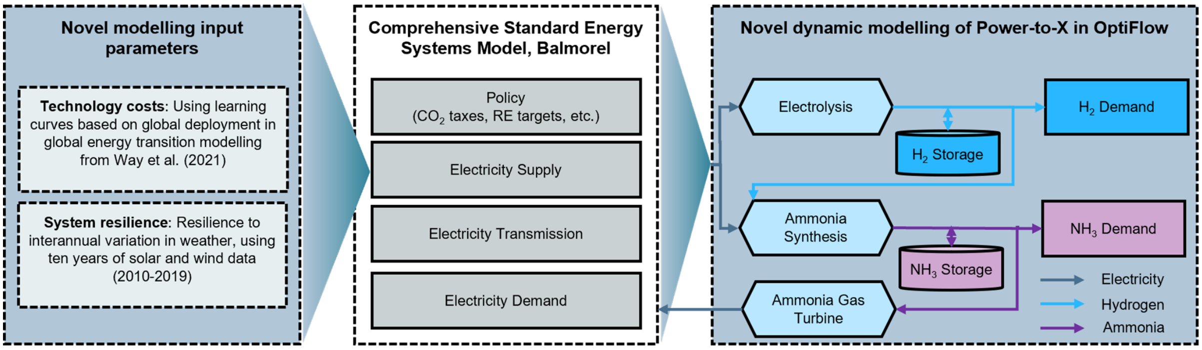


Figure 4.1: Overview of improvements to standard ESM.

The EEIST consortium is developing the ROA to address this need for different policy appraisal options, specifically in the realm of the energy system transition. Through historical case studies, the EEIST consortium finds that CBA is not suitable for modelling transformational change, and indeed CBA would have not supported early policies in the energy sector's transformation, including successful development, cost reduction, and deployment of offshore wind in the UK, solar PV in Germany and China, and LED lighting in India [175].

PtX in India is an example of a sector which will cause non-marginal, *transformational* change to the electricity system, and therefore a good use-case of ROA for the EEIST consortium. The EEIST consortium posits that traditional CBA approaches to green hydrogen policy are not appropriate and would almost certainly miss the opportunities associated with investment in innovation in this field. The failure to recognise these opportunities causes large errors in modelling estimates of the cost and the best approaches for tackling climate change.

Some of the non-marginal effects of PtX on the system include significant changes to electricity planning and system operation (the focus of this thesis), changes to land and water use, geographic and operational labour changes, significant reduction of imported energy, and significant potential for exported energy. While the ROA is still under development as part of the EEIST project, three ROA approaches have been used in this research to improve upon traditional energy modelling approaches. Specifically, the three areas which traditional ESM fall meaningfully short which are improved in this thesis are (i) complexity modelling (e.g. sector coupling and network-effects), (ii) positive feedback loops (e.g. learning-by-doing cost curves based on experience), and (iii) system resilience to uncertainty.

4.4.1 Complexity modelling: Ammonia and hydrogen sector coupling and networks

The first innovation is sector coupling of the power, transport, and chemical sector based on OptiFlow. This network includes hydrogen and ammonia production, storage, transport, and use in steel, maritime fuel, FCEV, fertiliser, and re-electrification in the power sector. As highlighted in the previous literature review sections, the chemical sector (e.g., fertilisers and steel) and heavy duty transport (e.g., shipping fuel, aviation fuel) are often overlooked. For the ESMs which do include these sectors, there is a gap in modelling flexible ammonia synthesis with ammonia storage options. The techno-economic assumptions, India specific demands, and transport infrastructure network potential are included in Chapter 4.

Of course, there are limitations to this OptiFlow/Balmorel model used in this thesis as well. First, thermal sector coupling (heating and, more relevant in India, cooling) are not modelled in detail. The load for cooling is included in the electricity demand, and the seasonality of the profile is somewhat captured; however, the potential for smart operation of residential, commercial, or industrial heating or cooling is not considered. Similarly, EV demand is included in the overall electricity demand growth, but smart charging is not included. The exclusion of thermal and EV smart sector coupling likely causes this thesis to overestimate the need for short duration batteries. However, since the focus of the work is on long-duration storage and the role of ammonia, it is an acceptable limitation. In the chemical sector, aviation demand is not included, as forecasts for hydrogen based aviation demand in India to 2050 are very uncertain. The technological pathways are still unclear, for example between DAC-based synthetic fuels and biofuels. Therefore, it was considered more conservative to exclude aviation from this thesis's modelling. Other chemical sectors with potential for flexibility, like aluminium, paper, cement, etc. also were not included due to a lack of data. Steel production flexibility and storage was not considered, as the flexibility and costs of the green hydrogen based steel production process still have to be better understood. These additional chemical sectors and flexibility should be included as their techno-economic potential becomes clear.

4.4.2 Learning-by-doing: Technology Experience Curves

The second innovation is using empirically grounded technology cost forecasts (experience curves) based on global energy transition scenarios from Way et al. [137]. Experience curves are a reliable forecasting tool for technology progress [177] and have been found to be significantly more reliable than expert forecasts in the context of the energy transition [135]. Many technologies, such as solar PV and wind turbines, decrease in costs as they are scaled up in deployment according to a predictable experiential learning rate [178]. Way et al. [137] provide a compelling case for using experience curves to forecast cost declines in wind turbines, solar PV, batteries, and electrolysers when forecasting renewable electricity related costs in ESMs. Their approach is to use either Moore's Law or Wright's Law with a historically derived learning rate. Moore's law is exponentially based on a technology specific learning rate and dependent only on time; however, it faces more criticism as it assumes inexorable progress, regardless of policy, R&D, and physical limits [137]. Wright's law, on the other hand, is exponentially based on a technology specific learning rate which is dependent on quantity of the technology deployed. This allows Wright's law to consider experiential learning based on "learning-by-doing", rather than solely the passage of time. This is relevant for wind and solar PV, as it may be more sensible to assume that they will not continue their dramatic price decreases in 30 years as they become the majority of the electricity system and deployment slows [179].

Leading energy system models, such as those from the International Energy Agency (IEA) [23] [180] use cost estimates which are systematically biased against progress in key clean energy technologies [13]. Over the last ten years the IEA cost forecasts have resulted in abysmal modelling forecasting, specifically due to the rapid (but predictable) cost decline of solar PV, as shown in Figure 4.2[181]. Reliable and coherent cost forecasts are essential for predicting the transformation of an energy system. As shown in Figure 4.2, the outcomes of the ESMs are drastically different for the IEA based cost curves as compared to the learning-curve based cost curves of Way et al. [179]. Similar results can be observed in the case of India. For example, Lu et al. [126] forecast Indian solar capital costs to be \$550 to \$1,650 kW^{-1} by 2040, while the cost as of 2020 was \$596 kW^{-1} and still rapidly dropping [136]. Unsurprisingly, Lu et al. design an Indian electricity system which is dominated by onshore wind, rather than solar PV, amongst other differences with this thesis's study.

In this thesis, three global scenarios for the speed of the energy transition are considered (Historical Mix, Slow, Fast) from Way et al. [137] global transition modelling. The costs from Way et al. [137] are global median values which are then adjusted to India's specific percentile in the global mix (lowest 5% in solar PV costs and average for onshore wind). India is assumed to be at the median for battery and electrolyser costs. The Indian costs derived from Way et al.'s global transition scenarios are shown in Figure 4.3. Also shown are the latest IEA cost projections for India specific costs in various scenarios. The IEA's latest projections generally falling in between the Historical Mix and Slow scenarios (Figure 4.3), suggesting that they are still pessimistic compared to learning-curve based cost projections. As a limitation, India is assumed to be a price-taker, meaning there is no feedback between the endogenously found

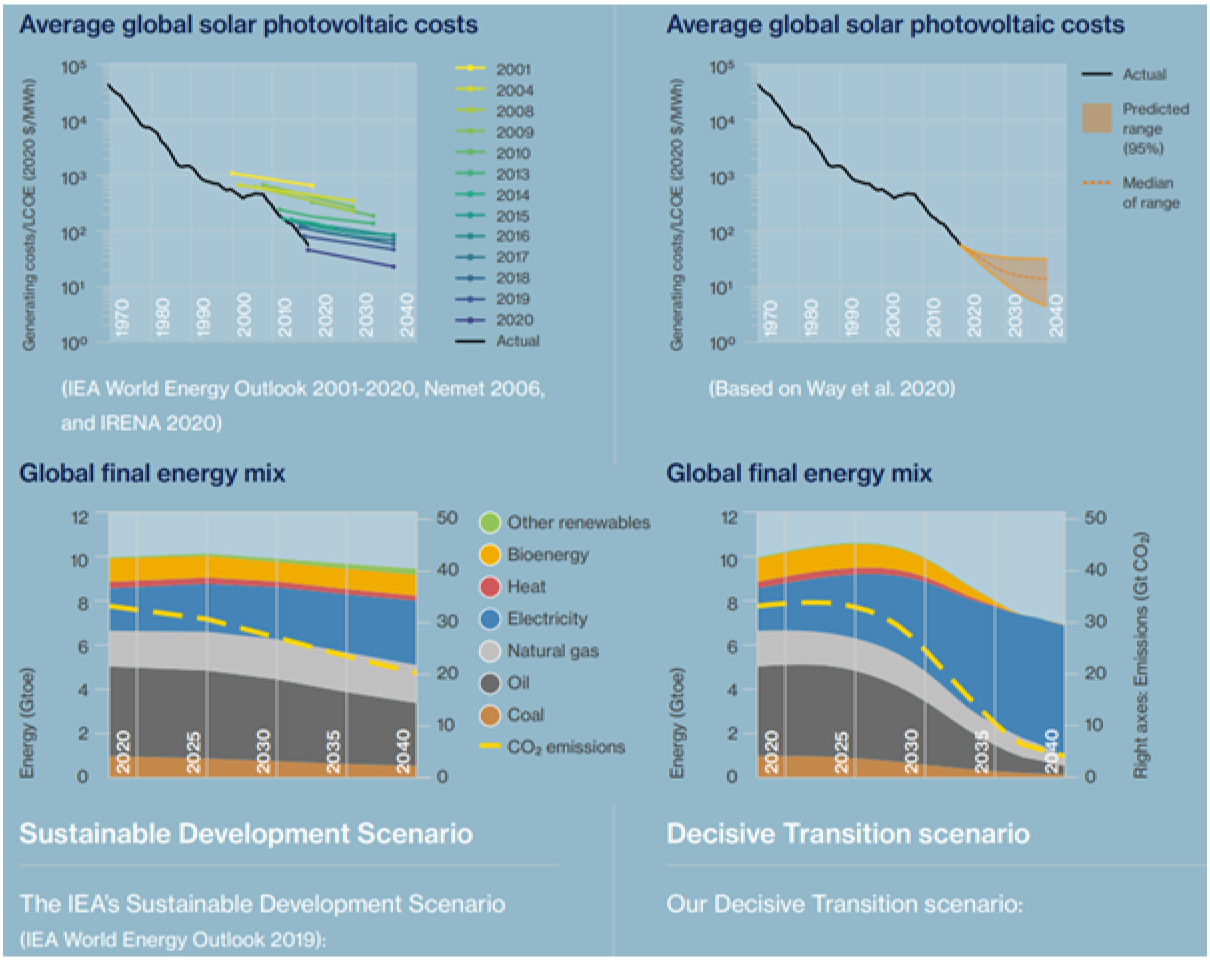


Figure 4.2: Top left: IEA based solar cost projections from various years which are reliably pessimistic and proven to be incorrect. Top-right: Way et al. solar PV cost projection based on learning curves. Bottom-left: IEA Sustainable Development Scenario global energy mix based on their cost forecasts. Bottom-right: Way et al. global energy mix based on learning curve cost forecasts in the Decisive Transition Scenario. Taken from [13].

deployment of technologies in the modelling and the global scenarios from Way et al. India is a very large market, so this assumption may not be completely defensible, but the complexity of feeding the deployment back into Way et al.'s global model was too high. Including this feedback would likely causes faster deployment levels and cost reduction, as even the Historical Mix scenario cost curves result in very high levels of RE technology deployment in India. India deploys RE technologies rapidly because they are cost competitive, even in the Historical Mix scenario, with the relative high cost of imported LNG and dirty coal power (with any level of CO_2 taxation).

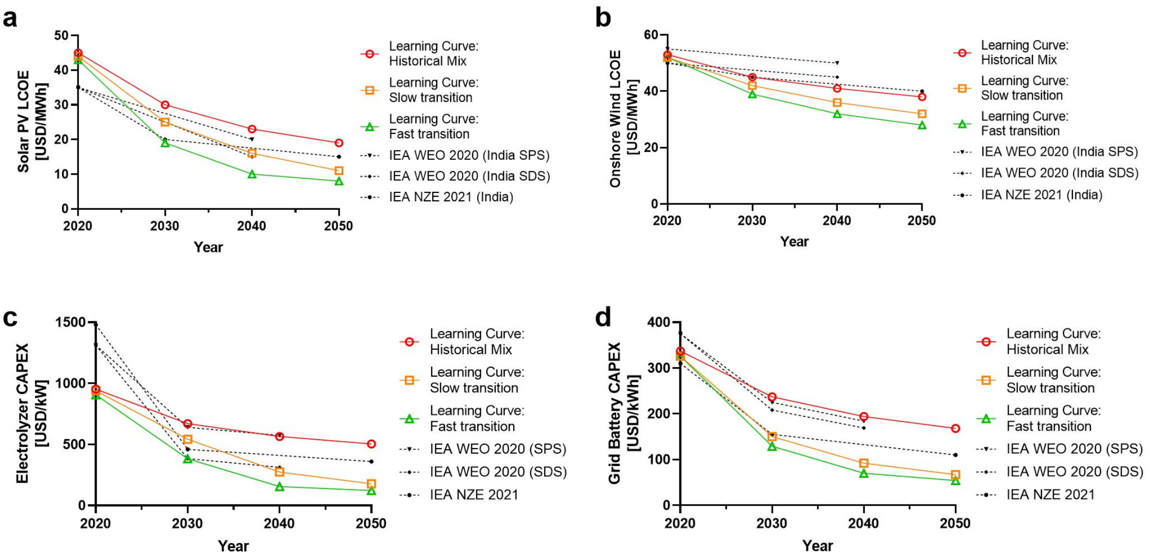


Figure 4.3: Cost reduction scenarios for key technologies, with comparisons to two scenarios from IEA World Energy Outlook (WEO), namely the Sustainable Development Scenario (SDS) and Stated Policy Scenario (SPS) [180], as well as comparison to the Net Zero Emissions by 2050 Scenario (NZE) [23]. India specific estimates used from the IEA for a and b, while global estimates used for c and d.

4.4.3 Modelling Resilience in Energy Systems via Multi-Year Wind and Solar Profiles

The third innovation is system resilience to interannual weather variation by using multiple years of hourly wind and solar data. An important part of the ROA [175] framework is to consider risks as well as opportunities. One key risk to future electricity systems with high VRE penetration is system resilience to uncertainty, shocks and tail-end probability events. These events can frequently be seen throughout the electricity systems of the world, such as recently in the Texas cold weather event in 2021 which caused catastrophic failure of the electricity grid [182] as well as recent low wind in the UK in September 2021 affecting electricity prices and natural gas prices [183].

One approach used in this thesis to begin addressing these weather-related risks and system resilience is to model multi-year wind and solar profiles at high temporal and spatial granularity. Most models use Typical Meteorological Year (TMY) wind and solar data, at different levels of spatial granularity, to generate profiles for inputting into the ESM. TMY data represents the median meteorological conditions based on long-term data but misses variation in wind and solar resources. Indeed, Balmorel is set up to use hourly data over one year for wind and solar profiles, and this thesis had to develop a new model temporal structure for adding multi-year profile capability. As detailed in the following section, variation in the last 40 years of re-analysis data for India finds monthly variation of ±35% year-on-year for onshore wind and ±10% for solar PV, which affects system design significantly. In the literature, Dowling et al. [104] find that including more years of weather data dramatically increases the need for long-duration storage in ESM results due to interannual variation, highlighting the relevance of this improvement to the ESM for the research questions of this thesis.

The following section details the methodology and validation for generating multi-year, spatially detailed hourly solar and wind profiles for use in the ESM.

4.5 Methodology: Generating accurate solar and wind profile data input for the ESM

The Balmorel ESM requires geographic specific hourly data input for renewable resources. Since this research is specifically interested in long-term electricity storage and dispatchable electricity generation from ammonia, seasonal and interannual variation of renewable profiles are important factors to capture in the data input. However, the vast majority of ESM reviewed use only one year of data.

Recent advances in climate modelling and satellite data have led to publicly available climate data sets at high spatial and temporal resolution. One of the most notable data sets is developed and maintained by the European Centre for Medium-Range Weather Forecasts (ECMWF), with the most recent version being ECMWF Reanalysis v5 (ERA5) [184]. ERA5 and its predecessor versions have been used by prominent analyses, such as the Intergovernmental Panel on Climate Change (IPCC) [185]. ERA5 is a reanalysis model which combines modelling data with observational data from around the world [186]. The temporal resolution is hourly and spatial resolution is 31 km (0.25 degree latitude / longitude) with further 0.1 degree resolution available for some variables. Hourly data is available from 1980 to the present.

4.5.1 Wind data processing

Wind data is provided from ERA5 as wind speeds in the eastward (u) and northward (v) directions at 10 and 100 m [186]. For this research, wind speeds at 100 m were used to minimise error from scaling 10 m winds to the 100 - 120 m range of modern wind turbine hub heights. To transform (u) and (v) wind speed into a single wind speed, Equation 4.2 was used.

$$windspeed = \sqrt{u^2 + v^2} \tag{4.2}$$

A hub height of 120 m above ground level was used to match to the increasing of hub heights in the Indian context, as assessed by National Institute of Wind Energy (NIWE) [14]. Wind scaling using a log law was used to scale wind speeds from 100 to 120 m, as shown in Equation 4.3. The resulting factor for scaling from 100 to 120 m in open land (i.e. roughness length of $z_0 = 0.03$) is 1.023 times the wind speed at 100 m.

$$V_z = V_{z_{ref}} \times \frac{\ln \frac{z}{z_0}}{\ln \frac{z_{ref}}{z_0}} \tag{4.3}$$

where:

V_z = Wind speed velocity to be calculated at height z

z = height above ground level for velocity v

z_{ref} = reference height where reference velocity is known

z_0 = roughness length in the current wind direction, 0.03 for open agricultural land

The wind power curve is used to translate hourly wind speed to turbine output power. The power curve is specific to the turbine chosen, and is an optimised design parameter for the site's wind profile. NIWE uses an average power curve generated from the power curves of seven modern wind turbines which have recently been installed in India. The curve from NIWE was found to closely match the IEC Class III curves from GlobalWindAtlas [15](see Figure 4.4), corresponding to wind turbines typically used in lower wind speed areas. This aligns with India, where onshore wind speeds are generally in a low wind speed regime. For the India wind data, the NIWE power curve was used.

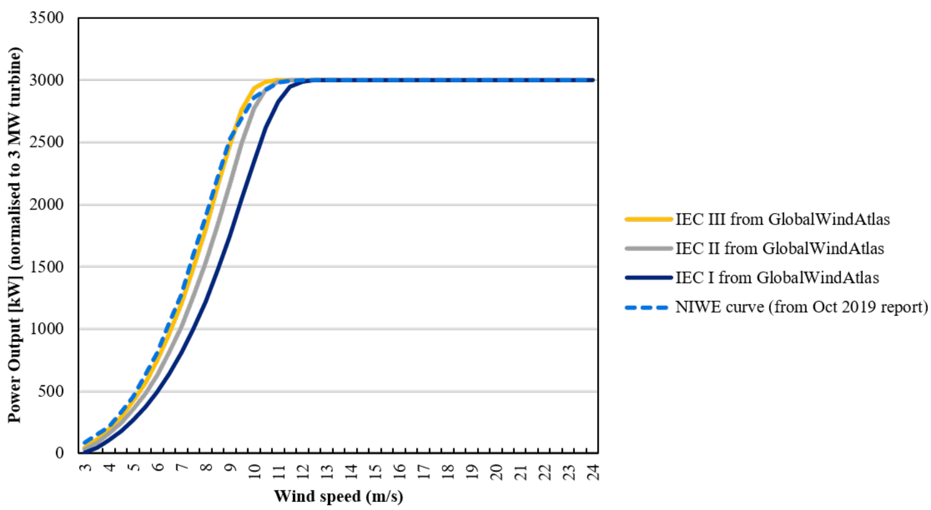


Figure 4.4: Wind turbine power curves, comparing NIWE [14] with IEC Class I, II, and III from Global Wind Atlas [15]

NIWE [14] analysed the maximum wind potential at 120 m for 35 states and union territories. This breakdown includes a breakdown of technical potential into five wind resource regimes based on Capacity Factor (CF). Of the resulting 175 potential regimes across all states and union territories, 85 have potential capacity, based on land use categorisation in NIWE [14]. Of the 85 possible pairs of wind regime and state or union territory, 48 were selected which captured 99.6% of the total NIWE resource potential, as shown in Figure 4.5.

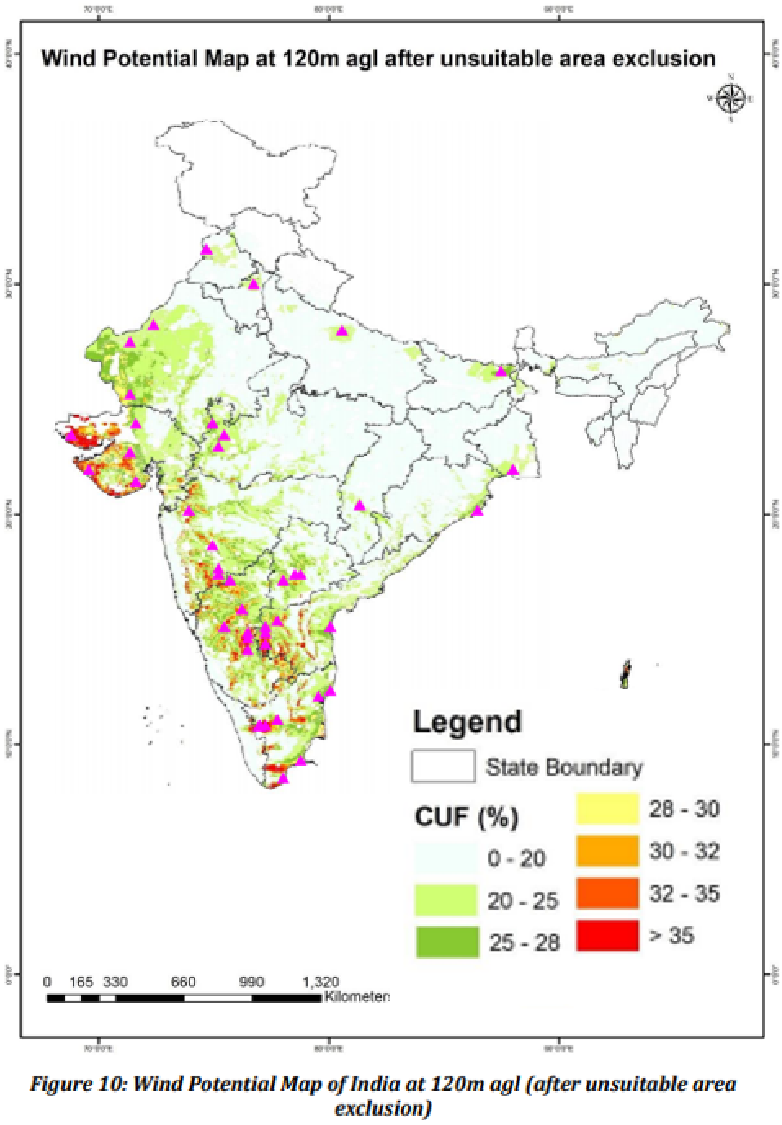


Figure 4.5: Wind locations and regimes from NIWE (background map with colour scale from [14]) and 48 locations (pink triangles) selected for ERA5 wind profile analysis

Using the methodology of translating ERA5 100 m wind speed to power output, the ERA5 results at the corresponding locations fit well with NIWE annual CF, based on an average of 40 years of (u) and (v) wind speed data at 0.25 degree granularity. A small correction factor was applied (see Figure 4.6), with a weighted average of 0.93, to ensure the ERA5 data matched the NIWE CF regime for each of the 48 locations. In some instances, the granularity of the ERA5 data was not high enough to capture certain wind regimes, based on topographical data; however the vast majority of features were captured by the ERA5 data.

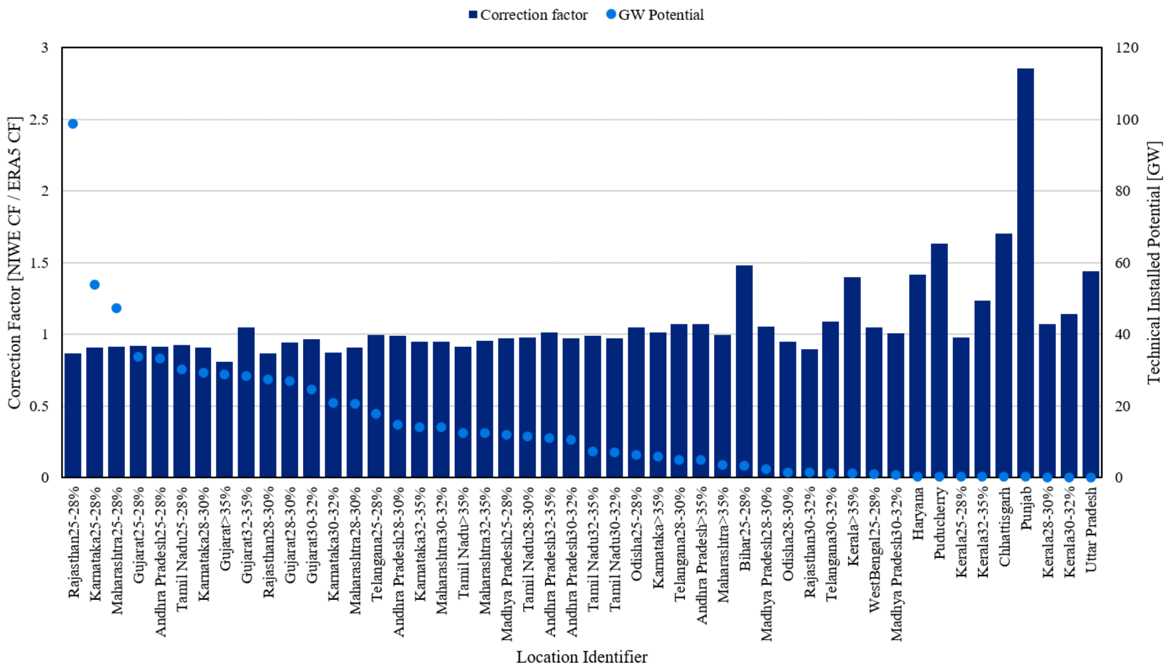


Figure 4.6: Wind CF correction factor across 48 locations from 40 year ERA5 average CF to fit in centre of NIWE CF wind regimes. Weighted average correction factor of 0.93. Locations are sorted from largest potential (99 GW in Rajasthan at 25-28% CF) to smallest potential (0.1 GW in Uttar Pradesh at 25-28% CF).

4.5.2 Wind data results

The maximum potential output of onshore wind power in India, based on 693 GW of installed capacity at 120 m on the sites identified by NIWE [14], is shown in Figure 4.7. The 40-year hourly profiles of 48 sites are generated using ERA5 hourly data from 1980-2019 and weighted according to the maximum potential installed capacity. In aggregate, the wind resource in India shows pronounced seasonality as well as interannual variability. Intra-annual variation (i.e. seasonality) is shown in stronger wind in monsoon season (June to September). Interannual variation is shown in the variation between various years from 1980-2019.

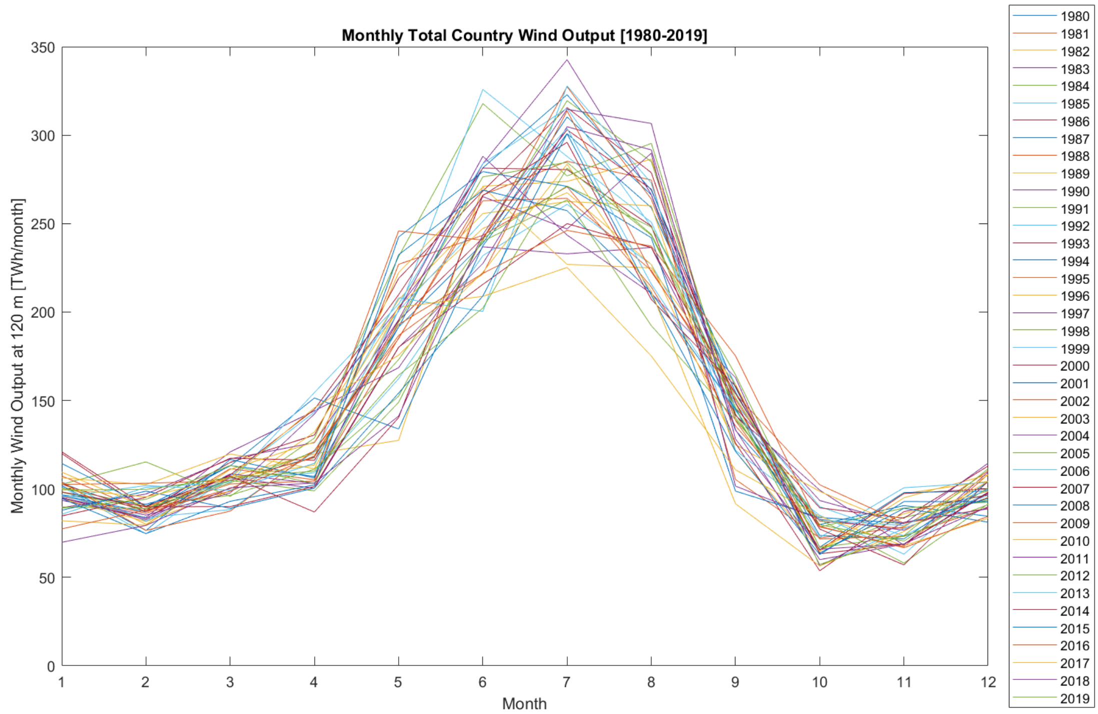


Figure 4.7: Wind power technical potential output of the entire country of India, based on NIWE 693 GW of installed capacity at 120 m and ERA5 hourly data from 1980-2019.

Interestingly, the data shows that annual onshore wind speeds are generally decreasing across all five electricity grid regions (Northern Region (NR), Southern Region (SR), Western Region (WR), Eastern Region (ER), Northeastern Region (NER)) (see Figure 4.8 for regional boundaries). This is corroborated by other studies finding a weakening of the monsoon [187]. The further trajectory of this decline is not considered in this work, but is an area for future work. As shown in Figure 4.9, interannual variation by region shows a maximum of ±20% variation from the 40 year average output.

In this research, daily energy storage is assumed to be economically met by batteries, while energy storage at a monthly, seasonal, and interannual level is the requirement of interest. Therefore, monthly variation results are analysed in more detail. Notably, the start of one month and the end of another month are arbitrary, and may hide further variation, but it was

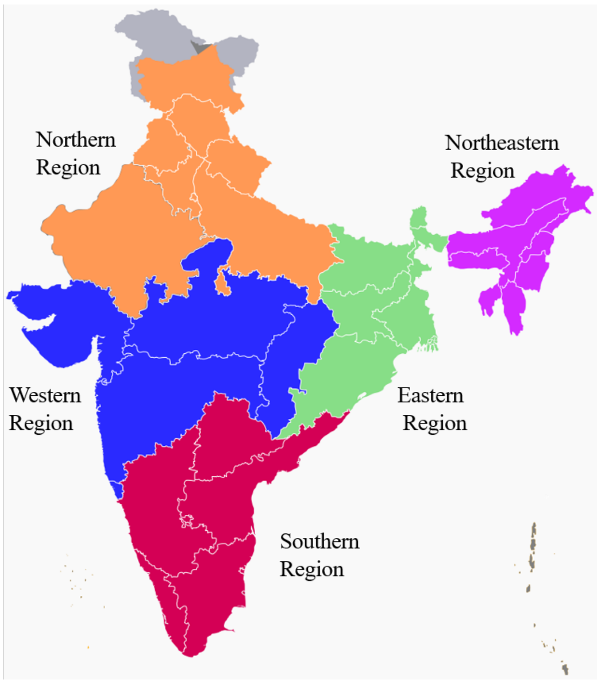


Figure 4.8: Five grid regions of India modelled in Balmorel ESM. Each region has unlimited transmission within the region, and fixed transmission capacity between regions, based on the historical grid structure in India. Background figure taken from [188]

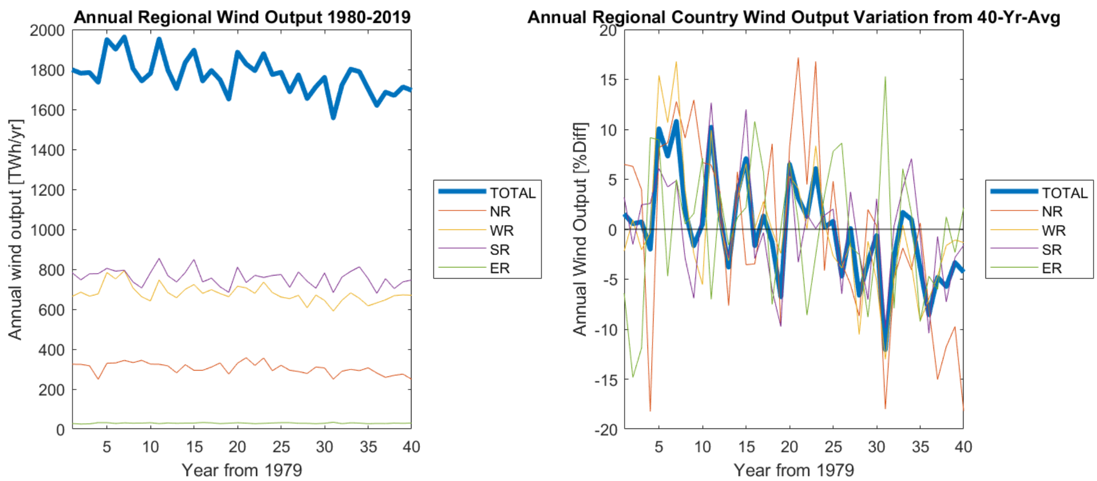


Figure 4.9: Left: Annual wind potential output over 1980-2019, with regional and aggregated totals shown. Right: Annual wind potential output over 1980-2019 as a % variation of 40 year average. NER excluded because very little technical wind potential is available in NER.

a useful analysis for a first pass and, in any case, Balmorel will optimise the system for costs using the full hourly profile. On a monthly analysis, the variation is shown in Figure 4.10 to be a maximum of ±35% year on year across all months of the year.

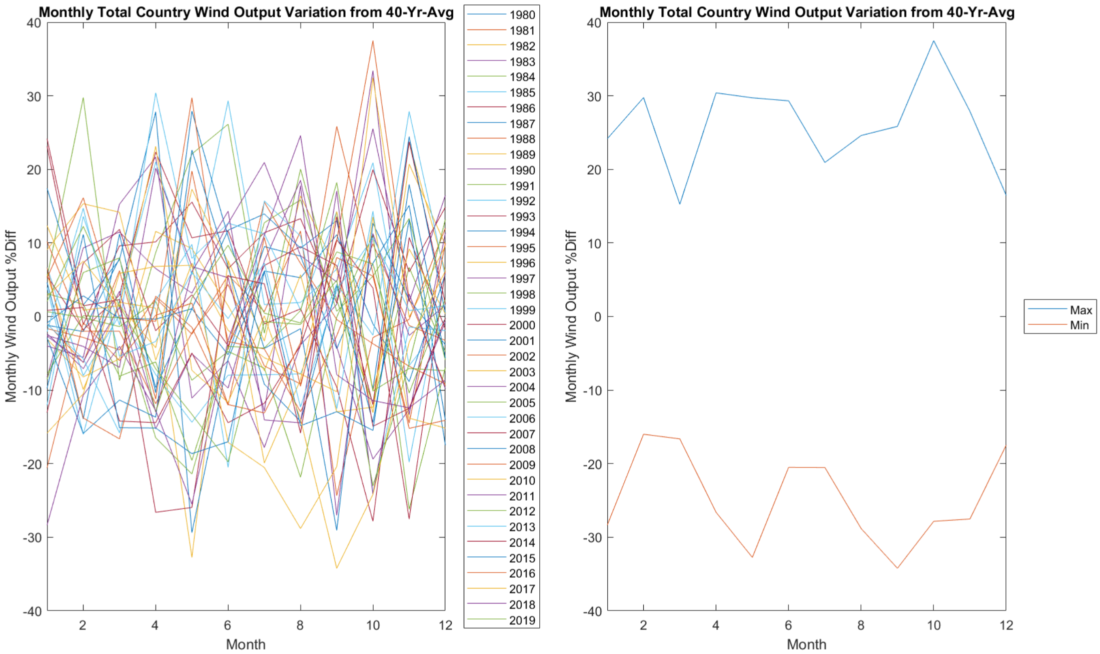


Figure 4.10: Left: Monthly wind potential output variation from 40 year mean. Right: Min and max of monthly variation from 40 year mean.

4.5.3 Solar data processing

Solar data is downloaded from ERA5 as Surface Solar Radiation Downward (SSRD), which is effectively Global Horizontal Irradiation (GHI) accumulated over 24 hour cycles [186]. Following the methodology of [189], ERA5 SSRD was transformed into PV output using the PVLIB Python open source toolbox [190] created and maintained by Sandia National Laboratories. SSRD is transformed into hourly GHI, then Direct Normal Irradiance (DNI) with consideration of the zenith angle at each hour at the given longitude, latitude, and altitude. With GHI and DNI, Diffuse Horizontal Irradiance (DHI) can be calculated. Finally, with GHI, DNI, DHI, temperature and wind speed, PVWatts modelling can be used to produce the hourly AC and DC power output.The data processing steps are outlined in Figure 4.11. While NIWE provides a very useful wind analysis of geographic specific technical potential, the National Institute of Solar Energy (NISE) of India does not provide a similar analysis of the solar PV technical

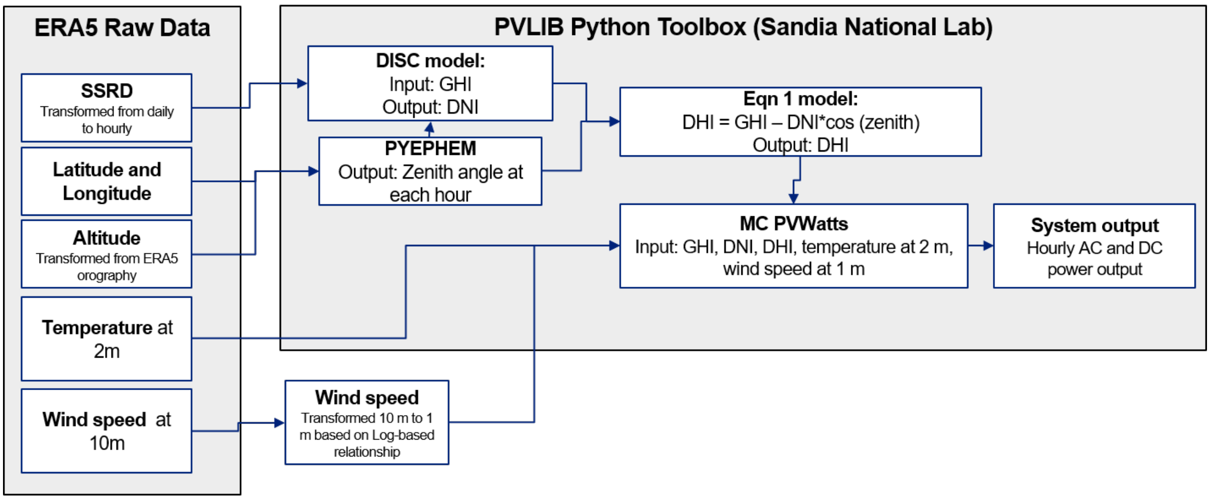


Figure 4.11: Data processing steps from ERA5 inputs to PV output using PV LIB.

potential in India. However, the National Renewable Energy Laboratory (NREL) offers a very useful tool, the RE Explorer, for calculating the maximum solar PV potential across India in granular geographic plots based on user defined land use restrictions [16]. This tool is used by The Energy and Resources Institute (TERI) in their recent analyses of RE uptake in India [132]. Using this data tool and land use categorisation which matches [132], 63 sites were selected which included all states at least once and enough solar profile regimes to capture any variation within states, as shown in Figure 4.12. Using the methodology of translating ERA5 SSRD to solar PV power output, the ERA5 results at the corresponding locations fit well with NREL annual CF. No correction factor was applied.

4.5.4 Solar data results

The maximum potential output of solar PV power in India, based on over 9,000 GW of installed capacity on the land identified by NREL as barren land, wasteland, and shrubland [16], is shown in Figure 4.13 (left). The 39-year hourly profiles of 63 sites are generated using ERA5 hourly data from 1981-2019 and weighted according to the maximum potential installed capacity. In aggregate, the solar resource in India shows pronounced seasonality with smaller

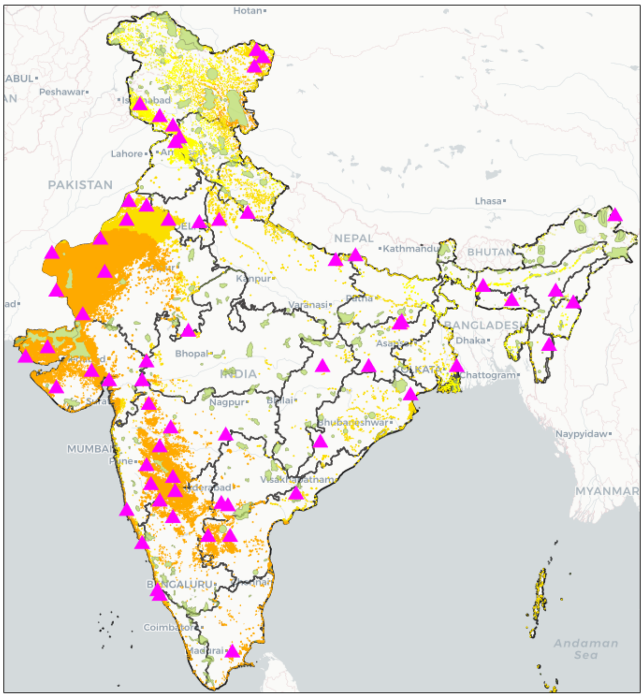


Figure 4.12: Solar locations and regimes from NREL (background map with colour scale from [16]) and 63 locations (pink triangles) selected for ERA5 solar profile analysis.

interannual variability than wind resources. However, aggregating data skews the results to the profiles of the NR, specifically Rajasthan, which accounts for 57% of the potential installed capacity. Intra-annual variation (i.e. seasonality) shows a peak in March to May, but again this seasonality is dominated by the weighting of Rajasthan's profiles in the aggregated data. Interannual variation is shown in the variation between various years from 1981-2019. Figure 4.13 (right) shows a variation maximum of $\pm 15\%$ variation from the 39 year average output, almost exclusively occuring in the monsoon months of June - September.

4.5.5 Wind and solar data validation

Real-world onshore wind and solar PV power plant data from individual power plants across India were gathered from publicly available monthly reports of the Central Electricity Authority (CEA) [17] from January 2020 to January 2021 to validate the ERA5 wind and solar profiles

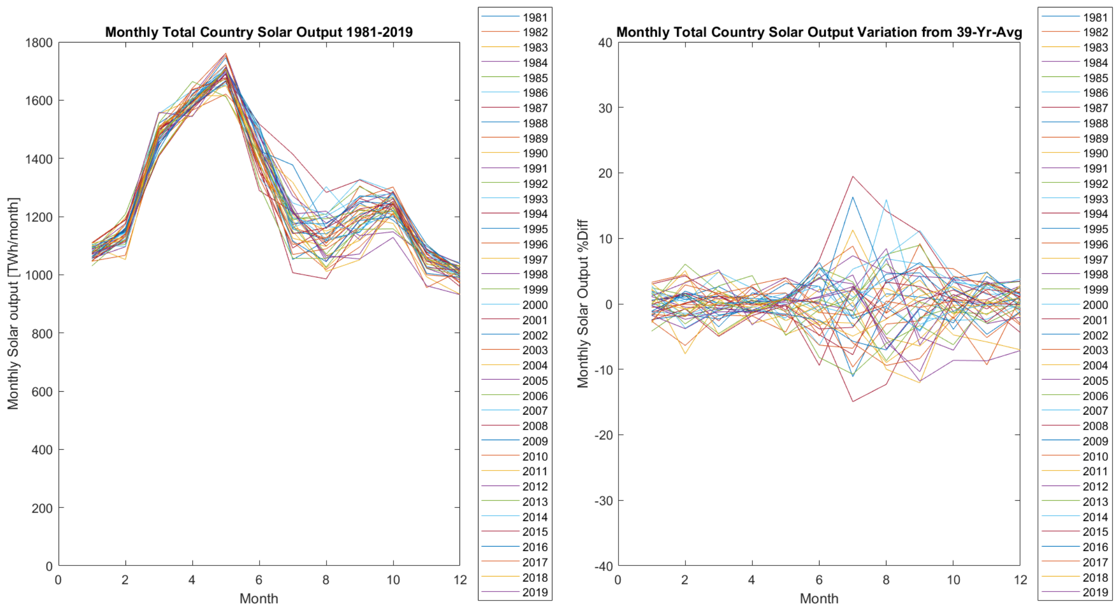


Figure 4.13: Left: Solar PV power technical potential output of the entire country of India, based on NREL 9,000 GW of installed capacity on barren and shrubland and ERA5 hourly data from 1981-2019 processed with PV LIB. Right: Monthly solar PV potential output variation over 1981-2019 as a % variation of 39 year average

and data processing methodology outlined in Sections 4.5.1 and 4.5.3, respectively. In total, 3.2 GW of wind power and 4.0 GW of solar PV power was represented with monthly level output. Wind power data is available on a monthly level for individual wind power plants across five states. These states account for 65% of the 690 GW of potential wind capacity in India. Solar PV power data is available on a monthly level for individual solar PV power plants across twelve states. These states account for 77% of the roughly 9,000 GW of potential solar capacity in India (with 57% of the capacity accounted for in Rajasthan alone). Overall, the validation analysis suggests that the shape of the wind and solar profiles used in this research are good representations of reality.

Unfortunately, some plant level data from CEA [17] has inconsistencies, plant shutdowns or curtailment, and erroneous data input. However, no post-processing was conducted on the CEA data in order to maintain the integrity of the validation exercise. Therefore, only plants with a full, coherent twelve month dataset were included. Manual matching of individual plant data was performed for a qualitative (visual) analysis to determine if the ERA5 data processing methodology reflects real-world conditions, as there is not enough spatial or temporal data (e.g. the data is lacking geographic coordinates and is only available at monthly time-steps) to perform a more rigorous quantitative analysis. However, the qualitative analysis performed still amounts to more validation than any modelling exercises in the literature today.

Wind

Analysis of the wind data suggests that the methodology outlined in Section 4.5.1 accurately represents real-world data, as shown in the comparison between real-world plant data and ERA5 processed data in Figures 4.14 and 4.15. Profile matching is shown for Madhya Pradesh, Maharashtra, Rajasthan, and Tamil Nadu in 4.14.

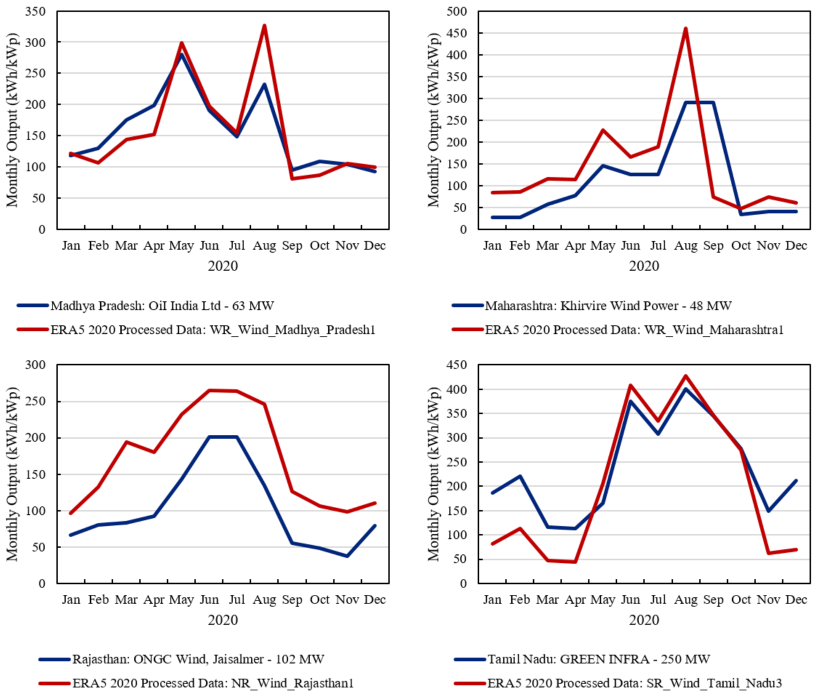


Figure 4.14: Real-world wind farm monthly output (blue) [17] with ERA5-based output (red) for individual wind farms in Madhya Pradesh, Maharashtra, Rajasthan, and Tamil Nadu in 2020. Longitude and latitude matching of sites cannot be confirmed due to a lack of data on individual plant geography; however, the qualitative state-level matching is very strong.

Figure 4.15 shows four individual plants in the state of Gujarat, at different locations within the state which experience different wind profiles. The locations chosen in the ERA5 process-

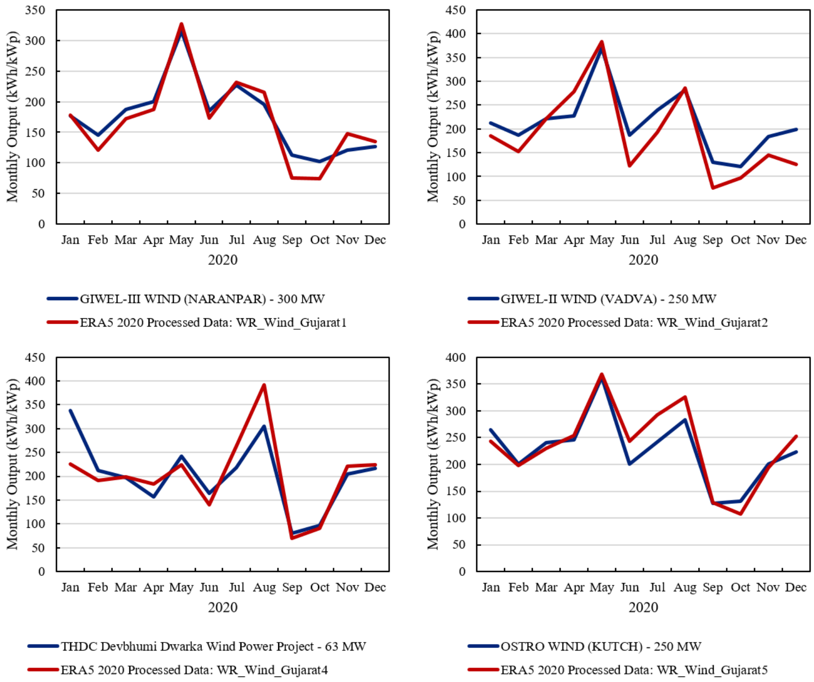


Figure 4.15: Real-world wind farm monthly output (blue) [17] with ERA5-based output (red) for four wind farms in Gujarat in 2020. Longitude and latitude matching of sites cannot be confirmed due to a lack of data on individual plant geography; however, the qualitative matching is very strong. As an exception, THDC (lower left) latitude and longitude was confirmed to match within 0.25° of the WR_Wind_Gujarat4 location.

ing for Gujarat, of which there are five, capture the profiles of each of these plants as shown by the close profile matching in the figure. Unfortunately, the geographic coordinates of the individual wind farms is not given in the CEA data and is difficult to find based on the information provided. One farm, THDC Devbhumi Dwarka Wind Power Project, from Figure 4.15, has been found based on publicly available data [191] to be located across seven villages clustered around [22.00°N, 69.75°E]. This geographic location is nearby wind location 4 in Gujarat, used in the ERA5 processing methodology outlined in Section 4.5.1, at [21.75°N, 69.75°E]. Therefore, it is further validated that the profiles match well with geographic accuracy, as shown in Figure 4.15, where the THDC project's profile is matched with Gujarat location 4 from the ERA5 data processing.

Solar

Similar to the wind data validation, analysis of the solar data suggests that the methodology outlined in Section 4.5.3 accurately represents real-world data, as shown in the comparison between real-world plant data and ERA5 processed data in Figures 4.16 and 4.17. Profile matching is shown for twelve states in Figure 4.16. While not all states match perfectly, the vast majority are close matches. Notably, the error in comparision to small size solar plants (e.g. 2 MW in Assam) should be discounted, especially compared to the accuracy of larger plants (e.g. 250 MW in Andhra Pradesh).

Figure 4.17 shows four individual plants in the state of Rajasthan which report monthly power plant outputs that have a similar shape to the ERA5 processed data, but uniformly higher. One explanation for this result is inconsistent rating reporting, as the capacity rating of the plant can be given in DC output (i.e. the electricity which the PV panels generate) or AC output (i.e. the output of the inverter system which transforms DC panel output into AC electricity for grid injection). To optimise costs, it is common to oversize the DC rating compared to the AC rating and curtail some power from the DC panels. This factor is named the Inverter Load Ratio (ILR), or ratio of DC output rating to AC output rating based on the sizing of the inverter. The result of reporting on AC rating in higher ILR scenarios would offset the output profile exactly as seen in Figure 4.17. Unfortunately, there is no data on ILR for these individual plants to validate this hypothesis. In any case, the shape of the profile is the most important factor for seasonal balancing, which is the focus of this research, and it appears to match fairly well with the ERA5 processed data for solar.

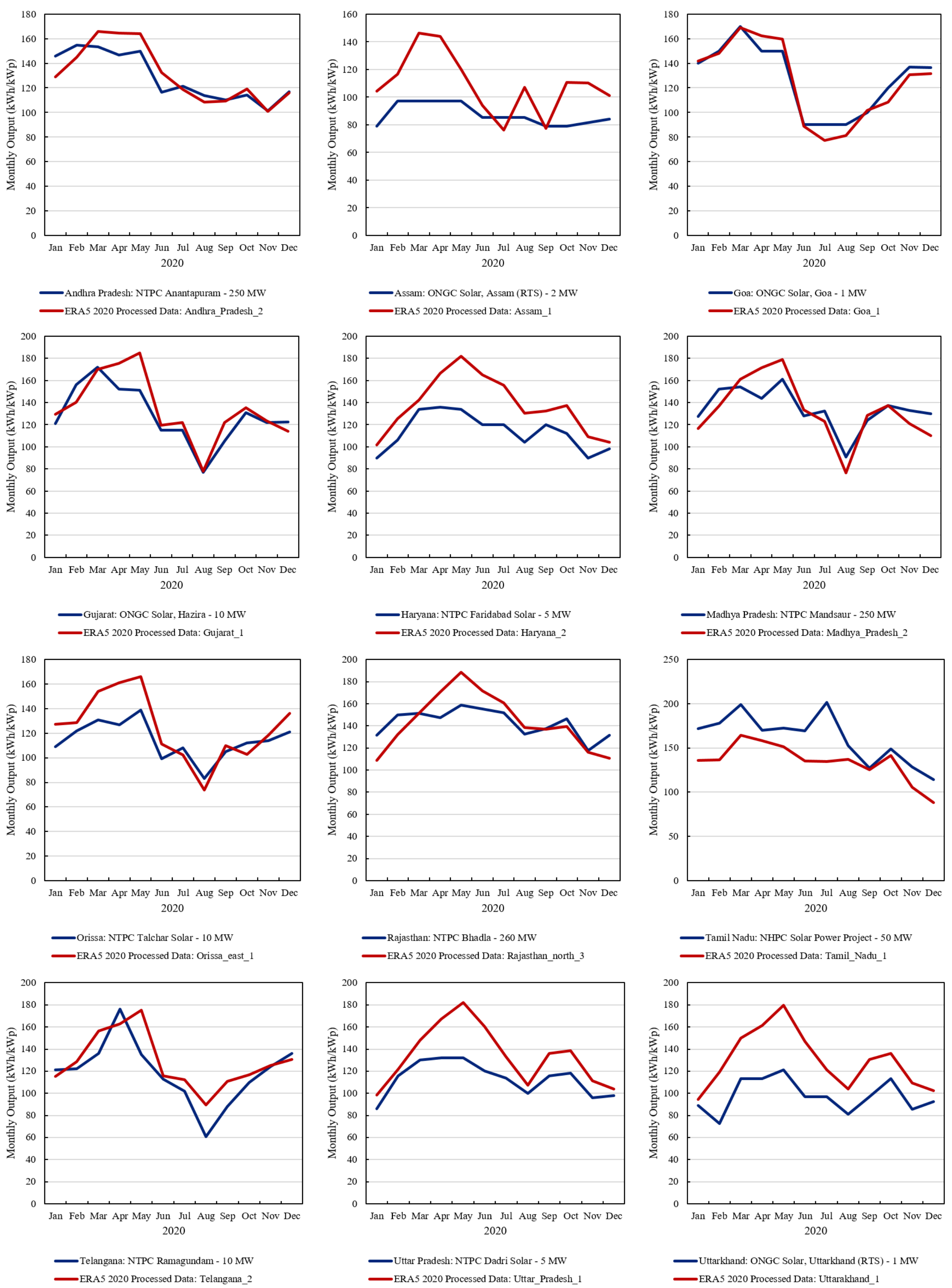


Figure 4.16: Real-world solar PV power plant monthly output (blue) [17] with ERA5-based output (red) for individual power plants in 12 states. Longitude and latitude matching of sites cannot be confirmed due to a lack of data on individual plant geography; however, the qualitative state-level matching is very strong.

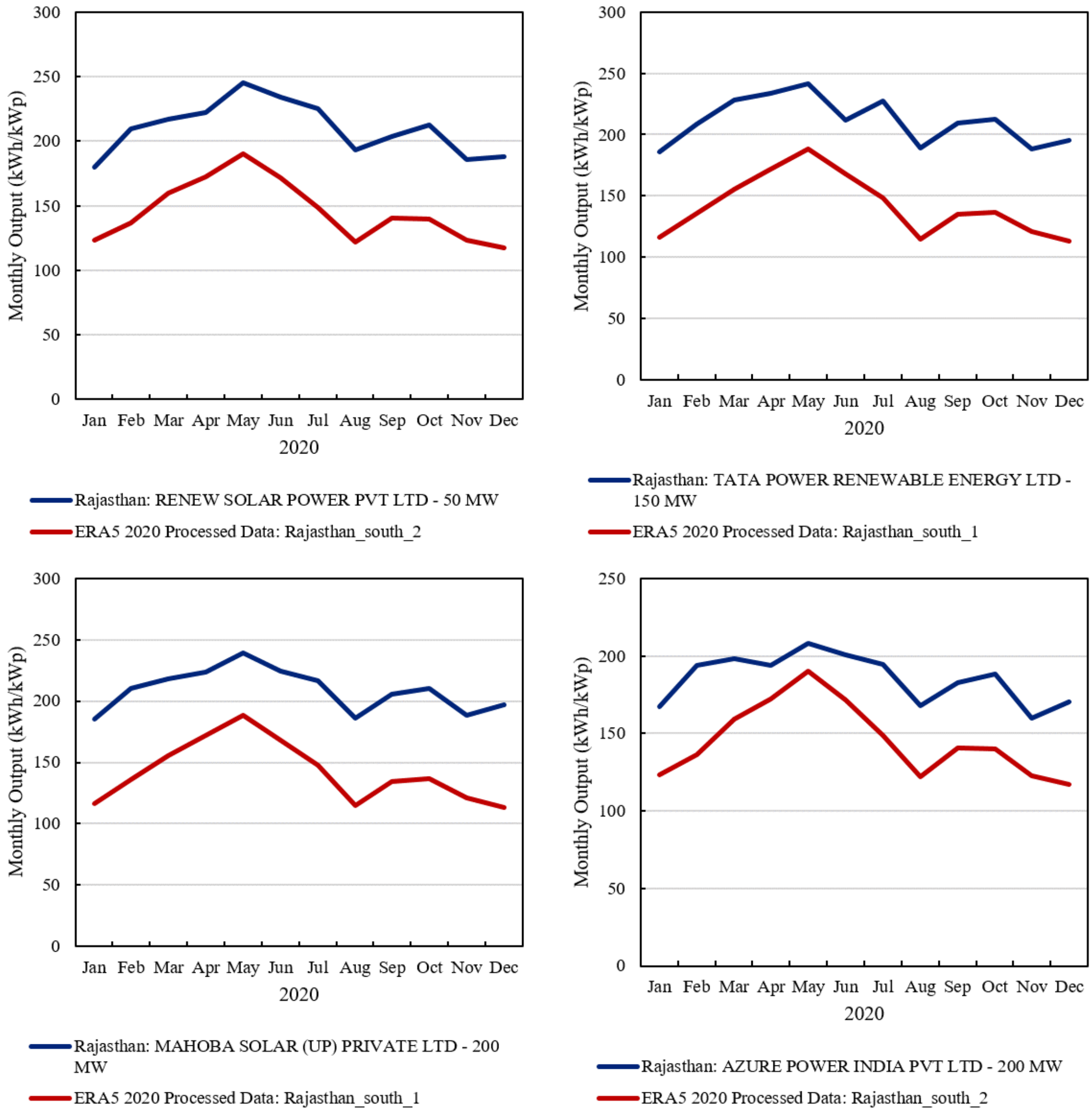


Figure 4.17: Real-world solar PV power plant monthly output (blue) [17] with ERA5-based output (red) for four power plants in Rajasthan which show an offset. This offset is likely due to ILR effects and reporting AC versus DC output; however, the qualitative matching of the shape of the profile is still very strong, which is most important for this research on seasonal electricity balancing.

5 | Case Study: the roles of green hydrogen and ammonia in India to 2050

5.1 Introduction

Overall, the objective of this chapter is to detail inputs to the ESM and present the results of the case study of India which is used to examine the research question on the role of green ammonia in decarbonised electricity systems, and address all three sub questions.

The objectives of this chapter are: (i) to provide the key data inputs for the model, including a deeper dive into the PtX demands in India, and (ii) to present the results of the ESM.

This chapter is segmented into three main sections: (i) a review of the sectoral PtX demand forecast in India, (ii) other key data inputs to the ESM, and (iii) the results of the ESM.

5.2 Sectoral demands for PtX in India

As described in Chapter 1, India is on the precipice of massive demand increases in the relevant sectors for this thesis's research questions, namely electricity, hydrogen, and ammonia. Today, India's grey hydrogen demand is approximately 6 MMTPA, or 8% of global demand, which is used roughly equally for refining and ammonia fertiliser production [2]. Already, the green hydrogen target announced in February 2022 as part of the NHM is 5 MMT by 2030 [18]. This target is not clearly stated as a cumulative or annual production target, but if it is annual, it is slightly more ambitious than this thesis's projections in 2030, as shown in Figure 5.1. Despite this early potential discrepancy, the demand forecasts of this thesis were not adjusted and modelling not re-run upon the recent government announcement, as the long-term quantity is more relevant for the research questions.

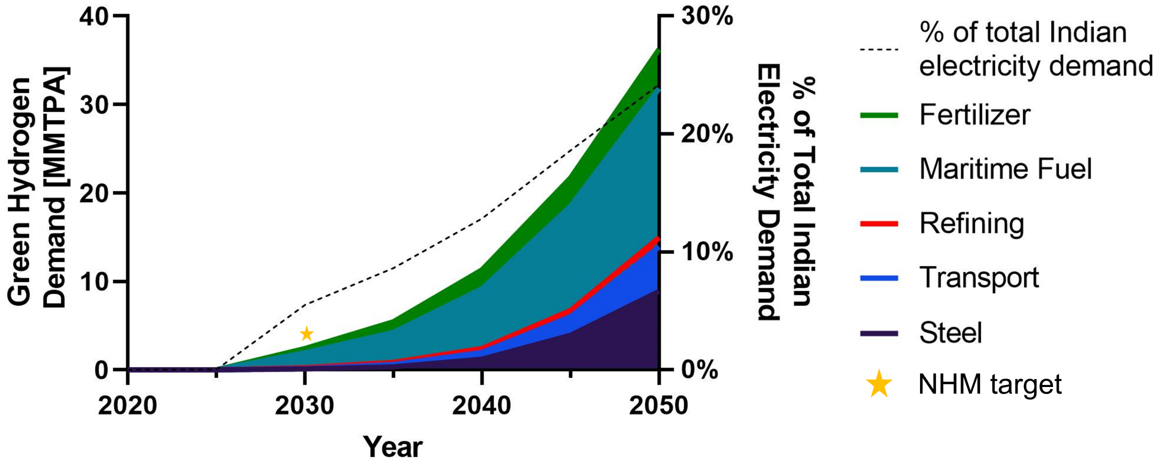


Figure 5.1: Green hydrogen demand scenario in India to 2050 by major end-use sector, including NHM target of 5 MMT by 2030 [18]. and the total percentage of India's electricity demand which is hydrogen production.

Table 5.1: Electricity, green hydrogen, and green ammonia forecasted demands in India to 2050

Year	2020	2025	2030	2035	2040	2045	2050	
Green Hydrogen Demand								
Steel	0.0	0.0	0.1	0.4	1.2	3.9	8.9	MMTPA H_2
Transport	0.0	0.0	0.0	0.2	0.8	2.1	5.0	MMTPA H_2
Refining	0.0	0.0	0.1	0.3	0.4	0.7	1.0	MMTPA H_2
Green Ammonia Demand								
Shipping Demand	0	0	10	19	38	67	95	MMTPA NH_3
Fertiliser Demand	0	0	3	7	12	18	25	MMTPA NH_3
Total Green Ammonia Demand	0	0	12	26	50	85	120	MMTPA
Green hydrogen and ammonia electricity demand								
Steel	0	0	5	17	56	181	412	TWh/yr
Transport	0	0	2	11	36	98	233	TWh/yr
Refining	0	0	5	12	20	32	47	TWh/yr
Shipping Fuel Demand	0	0	78	152	303	531	758	TWh/yr
Fertiliser Demand	0	0	22	55	96	144	199	TWh/yr
Total electricity demand for H_2 and NH_3	0	1	112	246	512	985	1649	TWh/yr
% of total Indian electricity demand	0%	0%	6%	9%	13%	19%	24%	%
Electricity Demand by Sector								
Agriculture	204	187	198	209	248	226	259	TWh/yr
Industry	419	622	810	1035	1278	1487	1784	TWh/yr
Transport	0	0	72	231	463	760	958	TWh/yr
Commercial	270	369	474	716	914	1057	1151	TWh/yr
Residential	187	270	369	413	578	777	1013	TWh/yr
Hydrogen and Ammonia	0	1	112	246	512	985	1649	TWh/yr
Total	1079	1449	2034	2851	3993	5292	6815	TWh/yr

This thesis uses an aggregate demand of almost 40 MMTPA of H_2 by 2050 (Figure 5.1). This section outlines the bases of the demand projections for each sector in Figure 5.1, i.e., steel, transport, refining, maritime fuel, and fertiliser, which are summarised in Table 5.1. Many of the base assumptions come from the "Low Carbon" scenario in TERI's seminal H_2 report [2], with the maritime fuel assumption coming from the most conservative scenario for India's contribution to fuel production in a net-zero shipping by 2050 World Bank report [3].

5.2.1 Fertiliser

As previously highlighted, ammonia's main use today is to produce nitrogenous fertilisers. Over 180 MMTPA are produced worldwide, with 18 MMTPA, or 10%, produced in India. Two factors create a large demand pull for new green ammonia production for fertiliser in India: the fertiliser market in India is rapidly growing, and yet it is largely dependent on imported ammonia and imported fossil fuels. Demand for fertiliser in India is growing, with estimates of total demand of Urea, DAP, and complex fertilisers increasing from circa 55 MMTPA today to 135 MMTPA by 2050 [2], as shown in Figure 5.2a. The per capita consumption is forecasted to increase from 45 kg to 75 kg, with the IEA's saturation level estimated at 85 to 135 kg per capita [2]. Today, India is the world's largest importer of ammonia, with imports equivalent to USD 1.3 billion [21]. Imported fertilisers make up 25-30% of India's consumption of fertiliser; however, even the domestically produced fertiliser is over 60% produced using imported LNG [68]. This reliance on imports is a major strategic reason for India to shift towards domestic green ammonia production for fertilisers. India is the fourth largest importer of LNG in the world [192].

In TERI's Low Carbon scenario, green ammonia plants are built from 2025 onwards and continue to displace aging natural gas plants and meet a growing demand [2], as shown in Figure 5.2b. By 2050, 60% of ammonia production for fertilisers is green. On the other hand, in TERI's Baseline scenario, only 33% of production is green by 2050 [2]. For this thesis, the

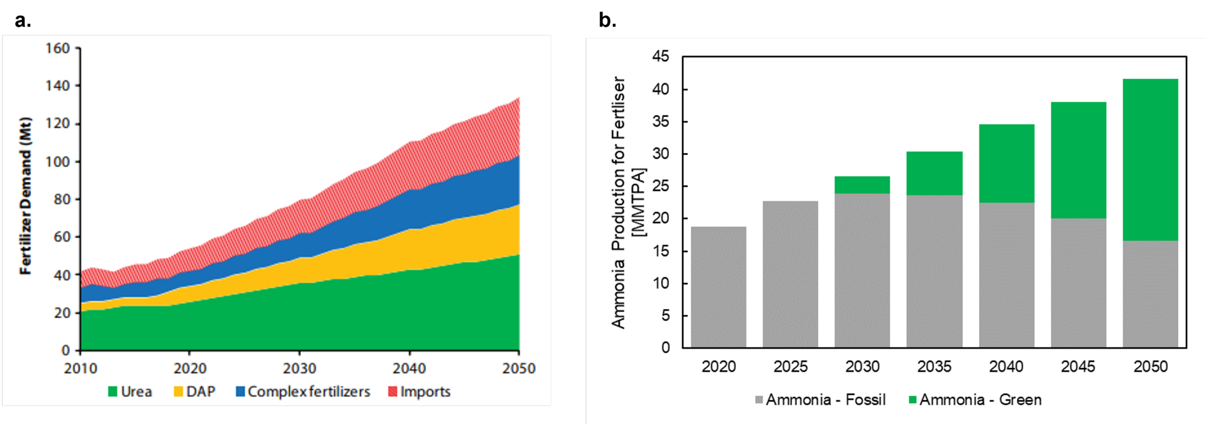


Figure 5.2: a. Demand for fertilisers in India 2010–2050 based on data from the Indian Ministry of Chemicals and Fertilizers, as aggregated by TERI [2], b. Grey and green ammonia production forecast in India in TERI's Low Carbon scenario [2].

Low Carbon scenario is used.

There are two key uncertainties that need to be highlighted in the shift towards green ammonia for the nitrogen required in the fertiliser industry. First, nitrogenous fertiliser is predominantly sold and applied to soils in the form of urea in India (see Figure 5.2a). Urea ($2(NH_3) CO_2$) is made up of two ammonia molecules and one CO_2 molecule. Today this CO_2 comes from a waste stream of the fossil-fuel-based Steam Methane Reforming (SMR) process. Unfortunately, this CO_2 is immediately released to the atmosphere upon application of the urea to the field and chemical reaction with water, so it is not a permanent form of CO_2 sequestration. Therefore, either green ammonia derived urea needs to use a net-zero compatible source of CO_2 from biomass or DAC, or a different nitrogenous fertiliser needs to be used. The IEA's roadmaps target shifting from urea to ammonium nitrate and Calcium Ammonium Nitrate (CAN) to eliminate CO_2 requirements for urea production [28]. Farmers' choice of fertiliser is influenced by many factors, including weather conditions, soil types and existing nutrient levels, crop types, existing and targeted yields, availability in regional markets, cost, subsidies, environmental regulations, handling ability and safety considerations [28]. These factors need to be further investigated in the regions of India. While some countries, especially the USA, use ammonia directly on the soil, this practise raises logistical challenges of transporting ammonia to farms, while solid urea is sold in non-toxic pellet form. The future final form for nitrogenous fertiliser in India is not clear at this point, but it is does not change the fact that ammonia will be the precursor nitrogen chemical in roughly the same quantity for whichever pathway is chosen.

The second uncertainty is the role of "zero-budget" farming practices, which do not use any input of inorganic fertiliser, and are becoming more common in India and indeed globally [193]. This technology is still in development, and therefore it is not clear what productivity is possible (and at what cost) compared with inorganic fertiliser applications. In the research to date, it seems that there will still be deficits of nitrogen in the Indian context even in the most optimistic forecasts of zero-budget farming in order to prevent decreases in yield [193]. Therefore, at this point in the technology development, it is prudent for this thesis's modelling to assume that nitrogenous fertilisers are still required and indeed demand will still grow. Indeed India's per capita fertiliser consumption by 2050 of 75 kg in TERI's growing ammonia demand model is still below the IEA's saturation level, estimated at 85 to 135 kg per capita [2].

5.2.2 Steel

India is the second largest producer and third largest consumer of steel today [194]. Moreover, India is a major demand growth market for steel looking forward to 2050, with steel demand growing three to fourfold from the large demand basis of 100 MMTPA today to 300 to 400 MMTPA [2]. Globally, steel demand is forecasted to grow 10-40% by 2050, increasing from 1,500 MMTPA of demand to 1,800 - 2,100 MMTPA, much of which is made up of Indian growing demand.

The global steel sector directly emits 2.6 Gt of CO_2 emissions per year via chemical process emissions, and 3.7 Gt per year in total when indirect emissions are included for the sector's electricity consumption. These emissions account for about 30% of direct industrial emissions and 7% of energy sector CO_2 emissions (including process emissions) [194]. The four major end-uses of steel are construction (50% of demand, including buildings, bridges, power plants, pipelines and sanitation systems), vehicles (15% of demand), machinery (20% of demand) and consumer goods (15% of demand) [194]. For most of these uses, there is no substitute material, and therefore significant primary steel production is regarded as unavoidable. Efforts to reduce the carbon emissions from the steel sector include scrap recycling and material efficiency. Material efficiency includes extending the lifetime of buildings, improving steel manufacturing yields, reducing steel content in vehicles and quantity of vehicles, improving building design, and reuse of steel (without remelting) [194]. Since it does not seem possible to replace steel, a carbon free production process is the current decarbonisation strategy. The three most mature technological pathways for reducing emissions to net-zero levels in steel production are Direct Reduction of Iron ore (DRI) with low-carbon hydrogen followed by Electric Arc Furnace (EAF) (henceforth "H_2 DRI-EAF"), direct reduction of iron ore using natural gas with carbon capture utilisation and sequestration (CCUS) followed by an electric arc furnace ("gas-based DRI-EAF with CCUS"), and carbon-based smelting reduction processes with CCUS and basic oxygen furnace ("SR-BOF with CCUS") [194]. The first pathway, H_2 DRI-EAF via green hydrogen-based production, has been demonstrated in the HYBRIT project in Sweden in 2021 [195]. The second pathway, gas-based DRI-EAF with CCUS, has been demonstrated in natural gas-based DRI plants in Abu Dhabi and Mexico, with a portion of CO_2 emissions captured and used for other industries [194]. The third pathway, SR-BOF with CCUS, has been demonstrated at the HIsarna project in the Netherlands, although it is not yet connected to CO_2 storage [194]. The competitiveness of the three routes depends on costs of local inputs (fossil fuels and renewable electricity costs), availability of CCUS, existing infrastructure, and CO_2 prices.

In India, using a cost of 2 USD/kg H_2, TERI found that H_2 DRI-EAF based steel would be produced at 350 USD/t, which is competitive with the current technology routes which produce steel at 300 to 500 USD/t in India [2]. The gas-based DRI-EAF with CCUS and SR-BOF with CCUS technology routes are less relevant for the Indian context because domestic gas is scarce, imported LNG is expensive, and CCUS geology is likely to be expensive or unavailable [2]. In the TERI baseline scenario, H_2 DRI-EAF based steel production is added to the technology mix starting in 2040, and only generates a H_2 demand of 1.5 MMTPA by 2050 [2]. In the Low Carbon Scenario, which is used as the input to this thesis's modelling, all new steel plants built from 2030 onwards are H_2 DRI-EAF based steel production, and thus 9 MMTPA of green H_2 demand is generated by 2050. This amounts to 50% of the steel production capacity in India in 2050, and therefore it is even possible to imagine a net-zero by 2050 scenario where this demand is twice as big. However, for this work, 50% decarbonisation via H_2 DRI-EAF based steel production is assumed.

Importantly, this thesis has not considered any flexibility in the steel production process. Therefore, any demand side flexibility in the model can only occur via hydrogen storage in aboveground tanks, which tends to be prohibitively expensive beyond intra-daily storage quantities. Further work should investigate flexibility in H_2 DRI-EAF based steel production and storing energy, in effect, in stockpiles of green steel, which could provide more cost-effective scenarios than those examined in this thesis.

5.2.3 Transport

The full transport sector accounts for 17% of India's total energy consumption [2], and 13.5% of India's energy-related CO_2 emissions [196]. Furthermore, the transport sector has been the fastest-growing energy demand sector in the last decades [68]. Since 2000, per capita rail travel and freight rail have doubled, truck freight has quadrupled with a thirteen-fold increase in the number of heavy freight trucks, and per capita vehicle ownership has grown five-fold [68]. India's total road network is now the second-largest in the world, behind the United States [68]. Since 2010, domestic aviation passengers have tripled and India has added 50 domestic airports in the last five years [68]. Shipping, covered in the following section, only accounts for 6% of freight transport; however, coastal and inland waterway freight shipping is expected to increase significantly in the coming years to reduce pressure on road and rail freight [2].

All these sub-sectors of India's transport sector are forecasted to continue growing by several-fold to 2050. The two main forecasts reviewed for this thesis are IEA [68] and TERI [2]. The IEA forecasts current transport sector demand increasing from 100 Million Tonne of Oil Equivalent (Mtoe) to 220 Mtoe by 2040 and, along a similar path, TERI forecasts 270 Mtoe (3,150 TWh) in 2050 for road transport. These values include electricity for EVs and hydrogen for FCEVs. There is large uncertainty in modelling these demands because, beyond the normal challenges with forecasting demand, policy and infrastructural choices will largely dictate the potential demand in each sub-sector. For example, in road and rail transport, different models and scenarios suggest different levels of potential growth, particularly in the split between transporting goods via truck or rail, depending on policy decisions [196].

In this section, the hydrogen demand for road transport is included (i.e., passenger vehicles, trucks, and buses) while rail, aviation and shipping are excluded. Shipping is covered using other analysis by the World Bank [3] in the subsequent section, but rail and aviation are excluded from this thesis's model of demand for electricity, hydrogen, or other synthetic fuels largely because detailed sub-sector analysis on the role of hydrogen could not be found in the literature for these other sectors. Rail is over 50% electrified in India today, and the government set a target of 100% electrification by 2023 [68]. Although this target will likely not be met, it shows the ambition to electrify completely in the near term. Thus, hydrogen will likely not have a significant role in rail transport in India. Aviation is excluded due to uncertainty around the technology pathway (e.g., biofuels versus synthetic aviation fuel versus hydrogen). This likely makes this thesis's demand scenario for hydrogen slightly conservative in 2050, but nevertheless the key results would remain unchanged.

The road transport sectors of trucks, buses, passenger vehicles, and two- and three-wheelers each need to be individually examined for estimating the proportion of hydrogen in future demand. Two- and three-wheelers account for 80% of road vehicles in India, but only 20% of fuel consumption, as they are more fuel efficient and travel lower distances [68]. TERI perform a Total Cost of Ownership (TCO) analysis on light-duty passenger vehicles as well as two and three-wheelers to find that BEV will be the most competitive option going forward, with hydrogen having a negligible share [2]. In heavy duty transport, i.e., trucks and buses, TERI finds a TCO analysis is more mixed, with BEVs more suitable for short distances (e.g. city buses) and FCEVs more competitive at longer distances (e.g. freight trucking and inter-city buses) [2]. The IEA is particularly bullish on truck freight driving the increase in overall demand for transport in India, accounting for over half of the demand forecast to 2040 in their models [68], so this use of hydrogen in decarbonising trucking may be a significant demand for hydrogen going forward which will need to continue to be updated with new techno-economic and real-world information.

One weakness of the TERI analysis is that hydrogen production is assumed to use grid electricity prices at the refuelling stations, assuming current electricity rates to 2050. This ignores any sector coupling potential or alternative hydrogen supply chain (e.g. liquid hydrogen delivery, or ammonia delivery with onsite cracking [197]) to reduce hydrogen price at the refuelling depot.

Given this high cost of hydrogen at the refuelling station, TERI only estimates that FCEV account for 5% of new truck sales and 10% of new buses sales in the 2050 Baseline scenario, which is increased to 27% and 13% respectively in the Low Carbon scenario [2]. In comparison, BEVs in trucks and buses account for 54% and 74%, respectively, of new sales in 2050 [2]. Furthermore, TERI assumes a significant role for Compressed Natural Gas (CNG) passenger and freight vehicles in 2050, which is quite surprising given India's dependence on importing LNG. The relative penetrations of the technologies in the two scenarios are shown in Figure 5.3, which clearly shows a very small role for hydrogen. Using this relatively low penetration of FCEV in buses and trucks, TERI's modelling results in 5 MMTPA of hydrogen in the road transport sector by 2050 in the Low Carbon scenario, with 4.2 MMTPA of this demand coming online after 2040 [2]. In the Baseline scenario, TERI only projects 1.5 MMTPA of hydrogen in the road transport sector [2].

In this thesis, the Low Carbon scenario was used, and even this is likely a conservative estimate of the potential hydrogen demand for road transport due to the pessimistic assumptions of hydrogen price at refuelling depots. In future work, the competitiveness of BEV versus FCEV will have to continue to be updated and the modelling updated accordingly, especially in the trucking freight sector.

5.2.4 Shipping

Many studies have looked at the various fuels for decarbonising the shipping sector, with ammonia and methanol as the leading candidates to date [29, 69, 70, 198, 199]. In most studies, ammonia has advantages compared to methanol due to the lower production costs as well as the uncertainty around CO_2 sources required for such a large production of methanol [29]. Bio-

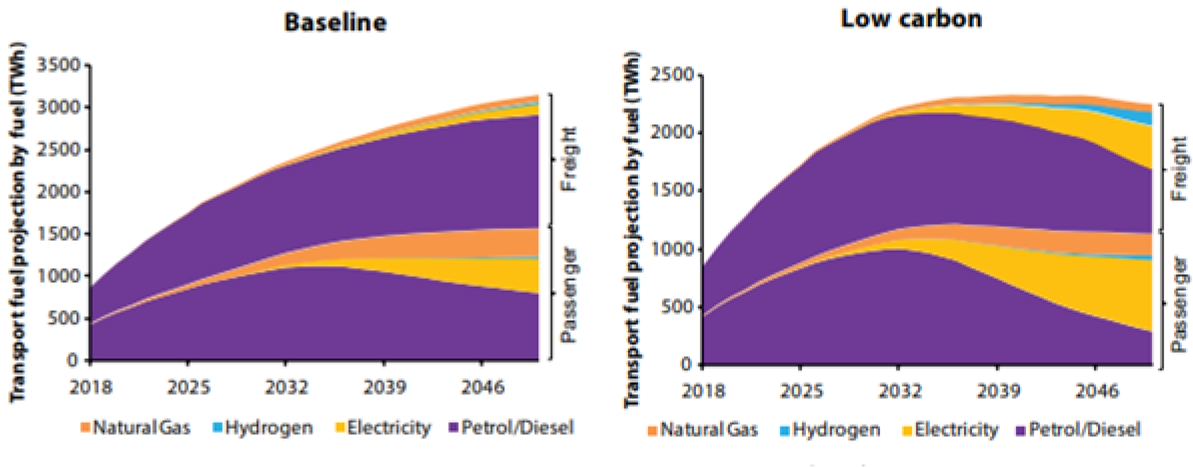


Figure 5.3: TERI [2] scenario analysis for road transport fuel in India by 2050.

fuels are largely not considered, or only considered for partial supply as they are unlikely to be able to scale to the level required for the shipping industry [29, 70, 199]. As further support for ammonia, shipping engine manufacturers are developing ammonia combustion engines, with MAN engines boldly claiming that an ammonia engine is 95% similar to existing engines and that they will have an ammonia engine on the market by 2024, with retrofits of existing engines available by 2025 [59]. Additionally, ammonia SOFCs are being scaled for a 2 MW shipping project by 2024 in Europe [94]. Finally, whether the fuel is green ammonia or methanol, the green electricity demand is effectively the same and the fuels have similar storage costs and process flexibility potential. Therefore, even if green methanol replaces some or all the share of green ammonia used for shipping fuel production in India, the results and findings of the ESM in this thesis would remain the same.

In looking at India, from modest beginnings today, there is a massive potential for producing green shipping fuel by 2050 due to large domestic demand increases, strategic location on major shipping routes, and large VRE resource potential, especially along the south, west, and north-west regions, which can be used for green fuel production. India is ranked 11th in the world in total annual container throughput via ports [3] and shipping accounts for 6% of the country's freight transport [2]. Today, India accounts for less than 1% of global bunker fuel sales [3] as there is relatively little oil in India, and it is used in other domestic markets. Looking forward, the policy emphasis of the NHM has been on replacing imports with domestic green hydrogen derived substitutes as well as creating large green hydrogen-based export opportunities [67], and providing bunker fuel to the global market would be one major export opportunity. India is strategically located on the major shipping routes via the Suez Canal which connect Asia, the Middle East, and Europe, and the shipping traffic can be seen in Figure 5.4 [3].

Figure 5.4: Shipping traffic 2015-2020 around India, from [3]

The shipping fuel scenario used in this thesis is based on World Bank's [3] scenarios for India's share on the supply of green ammonia in a 100% decarbonised shipping fleet by 2050. In the various scenarios, India supplies shipping fuel to the regions of Asia (which includes India's own shipping), the Middle East, and Oceania. In the lowest scenario, India supplies

25% of Asia's shipping fuel in 2050, totalling 95 MMTPA of ammonia and no fuel to other regions. In the highest scenario, India supplies 50% of Asia, 50% of the Middle East, and 50% of Oceania's shipping fuel to total 248 MMTPA [3]. The total global consumption of ammonia for shipping is estimated to be around 900 MMTPA by 2050 [3] and thus India would be supplying in the range of 10% to 28% of the global shipping fuel in these scenarios.

The more conservative 95 MMTPA was used in this analysis, limiting India's share to 25% of Asia's supply and thus 10% of global supply. This scenario was selected for several reasons. First, it is likely that other countries will compete in the Middle East and Oceania markets, given the vast VRE resources available at competitive prices in these regions and the clear signals towards leading the green ammonia world-scale production from Saudi Arabia [42] and Oman [200] in the Middle East and Australia [40, 41] in Oceania. Secondly, the sheer magnitude of India supplying 27% of global shipping fuel seems unrealistic to include in a model at this point, while 10% is already quite ambitious. This 95 MMTPA of ammonia is approximately five times larger than India's present-day ammonia fertiliser production capacity of 18 MMTPA. As shown in Figure 5.1, the shipping demand accounts for almost half of the hydrogen demand included in the model, so this assumption has a large impact on the modelled demands.

5.2.5 Refining

Hydrogen is needed in the refining of crude oil into gasoline, diesel and other products, as well as for desulphurisation. Today, refining of crude oil in India consumes 2.6 MMTPA of grey hydrogen. TERI's sectoral analysis on refining assumes 50% of hydrogen demand in refining is met by green hydrogen in 2050; however, the figures in the published report are contradictory regarding the total amount of green hydrogen that this requires. Specifically, Figure 1 from

[2] shows 1 MMTPA of green hydrogen in refining by 2050 while Figure 4 in [2] shows 4.5 MMTPA. In this thesis, the more conservative value of 1 MMTPA was used, partly because it is sensible that a Low Carbon scenario should require less total refining capacity than India's present demand for grey hydrogen in refining, which is 2.6 MMTPA [2]. Given the total size of the green hydrogen demand, this discrepancy is relatively small and therefore will not change the results of the analysis.

5.3 Key data inputs

5.3.1 Scenarios

In ESM, scenario analysis is a useful methodology for developing coherent plausible futures and exploring different policy decisions or technology developments. While it is impossible to predict the future, and no scenario will be entirely validated over the next decades, the scenario based analysis allows modellers to test variables and make somewhat informed decisions based on the scenario outcomes.

In this research, sub question 2 was specifically focused on the effects of connecting ammonia synthesis to the grid or having it islanded. Therefore, the scenarios modelled were split in either islanded or connected configurations to explore the effects on the overall system. In the islanded case, all hydrogen and ammonia electricity demands are met via dedicated VRE which is not connected to the electricity grid. In the connected case, the fleets of electrolysers are connected to the grid. 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 favour 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 shown in Figure 5.13c. Therefore, a large proportion of the costs of the connected scenarios should be captured in the form of new investment in transmission. Further work should explore grid connection charges and the underlying basis for adding them to future models. In any case, this scenario analysis comparing the connected and islanded extreme cases is illustrative of the different paths that could be pursued from a policy standpoint and some of the system operational and cost effects.

In addition, a major uncertainty which affects ESM results is the forecasted cost decline over time of key technologies, as highlighted in Section 4.4.2 Learning-by-doing: Technology Experience Curves. In this thesis, three global scenarios for the speed of the energy transition are considered (Historical Mix, Slow, Fast) from Way et al. [137] global transition modelling. In the three different transition speeds, the cost forecasts for solar PV, onshore wind, electrolysers, and short duration batteries are derived from the method of Way et al. [137] as outlined in Chapter 4 and shown in Figure 4.3. The costs from Way et al. [137] are global median values which are then adjusted to India's specific percentile in the global mix (lowest 5% in solar PV costs and average for onshore wind). India is assumed to be at the median for battery and electrolyser costs. Importantly, modelling technology costs using coherent global deployment scenarios ensures that the relative rate of cost decline amongst the technologies is defensible. Running these three scenarios is the equivalent of running a sensitivity analysis on the technology cost forecasts, but has a more coherent assumption than single technology sensitivity analysis. According to this logic, a technology, such as solar PV, does not change cost forecast without corresponding cost forecast changes in wind and batteries which would be deployed proportionally alongside it. Across all scenarios, other mature technologies (e.g., nuclear power, hydropower, fossil fuel based power generation) do not experience cost changes over time. This is consistent with Way et al. [137] which found that these technologies have plateaued in cost declines and therefore are unlikely to see further changes. If anything, some technologies, like nuclear, have become more expensive over time, and thus this assumption towards plateauing costs is conservative in regards to renewable penetration. On the other hand, new technologies, like small modular nuclear reactors, may allow for cost declines of nuclear in the future. Future work should update costs as significant changes occur or look likely to occur.

Using three different speeds of global transition for technology costs (historical mix, slow, fast) across two network configurations for power-to-X (connected or islanded), six scenarios are modelled to answer the research questions.

5.3.2 Spatial and temporal resolution

The ESM considers 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 National Electricity Plan (NEP) [201] and Electric Power Survey (EPS) [202].

The system's generation capacity expansion was modelled to 2050 in 10 year time-steps. ERA5 [184] climate data is used for generating hourly solar and wind profiles for 2010-2019 as detailed in Chapter 4. The most granular timestep is hourly, however an aggregation of every 5 hours and every 5 weeks was found to capture interannual weather variation as well as hourly weather variation without causing untenable calculation times.

The approach to modelling interannual variation was to consider 10 years of weather data for each 1 year of simulated operation. In effect, the least cost system chosen in the optimisation was the system which was least cost when operated over the 10 years of data, rather than just 1 year. In each simulated "year", 3,536 hours were simulated. These hours were selected first by only considering every 5th week over the 10 year weather data (i.e., week 1, week 6, week 11, ... week 516) which totals 104 weeks out of the possible 520 weeks of data. Then, within these weeks, every 5th hour is considered (i.e., hour 1, hour 6, ... hour 166) which totals 34 hours per week out of the total possible 168 hours. This time aggregation was found to adequately capture hourly variation, inter-daily variation, seasonal variation, and interannual variation across 10 years of weather data. In this configuration, the model runs took 3 to 72 hours on 256 GB RAM, 2.2 GHz. The variation in model run had to do with the connected versus disconnected scenarios (with connected taking longer to run) and the Historical to Fast costs (with Fast taking the longest to run).

Batteries were modelled with a fastest time to charge of 4 hours and fastest time to discharge of 4 hours, representing the most economic energy storage usage of batteries. Pumped hydro was modelled with an 8 hour fastest charge of storage and 6 hour fastest discharge. Longer duration storage batteries such as flow batteries were modelled in preliminary model runs with fewer timesteps, but were found to not be used and therefore were excluded from the final runs to save run time. In an ideal world, all types of technologies are included in the model; however, in practicality this increases run time and simplifications must be made to exclude technologies which are consistently never implemented in test runs.

Hydro seasonality was modelled using rainfall data for 1 year. In future models, this should match the 10 years of weather data; however, this limitation is likely small as hydro plays a relatively minor role in the final system design compared to wind and solar.

5.3.3 Green hydrogen and ammonia production and storage

Green hydrogen and ammonia production was modelled used electrolysers, aboveground hydrogen storage in tanks, flexible 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 [2]. Therefore, aboveground hydrogen storage in tanks was the only hydrogen storage technology considered in this analysis.

The production modelling of ammonia is typically modelled in islanded systems [6, 77], while more rarely modelled in grid connected scenarios [72]. 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 [78] 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 utilisation. 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 [78], 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 [79]. 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. All other process equipment (electrolysers, ASU) were allowed to ramp on and off with perfect flexibility, which does not perfectly mimic reality but is a reasonable assumption for the level of temporal granularity of this model.

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 [24]. Exporting green hydrogen and ammonia is a strategic target announced in the NHM [67], 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, subsidising domestic industries such as steel and fertiliser, etc.

Ammonia and hydrogen pipeline infrastructure was assumed to be available between all regions except the Northeastern Region (NER). Shipping infrastructure was assumed to be able to connect the WR and SR, as well as SR and ER. The NR does not have a port, and therefore pipeline is the only option from the NR. Distances are outlined in Figure 5.5.

Ammonia and hydrogen transport were only included for the exogenous demands (i.e., fertiliser, steel, maritime fuel, heavy duty vehicles, and refining), and not for the endogenous demands generated in the power sector. For the power sector, ammonia produced in any region is available for consumption in any other region. This mimics LNG availability in the model, which is modelled as one landed price for the whole country. Additionally, demands for ammonia-to-power are very small, from 0 to 10 MMTPA, in comparison to other ammonia demands (120 MMTPA), and thus the infrastructure required to move ammonia between

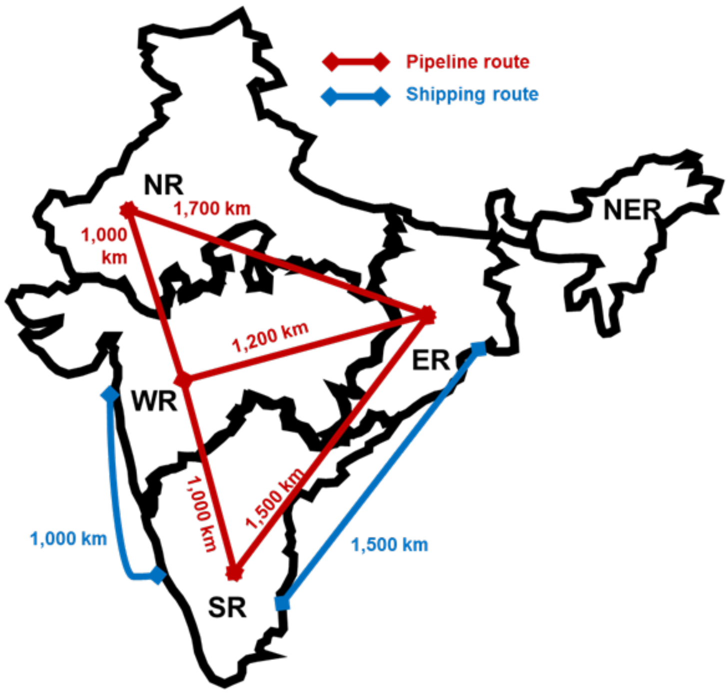


Figure 5.5: Pipeline and shipping potential infrastructure and distances assumed in the OptiFlow ESM which connects the Northern Region (NR), Western Region (WR), Southern Region (SR), and Eastern Region (ER). No connection is assumed to the Northeastern Region (NER).

regions for the power sector would be far smaller. This simplification greatly reduced model calculation time.

Green ammonia was included as a new fuel option to be used in CCGT power-plants. Due to the high cost of aboveground hydrogen storage, ammonia has significant techno-economic advantages for use in dispatchable GTs and there are clear signals from manufacturers to have ammonia-fired GTs on the market by 2024 [60]. 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 fertiliser and maritime fuel demands). Hydrogen GTs were not included in the model because of the impracticality of storing GT quantities of hydrogen in aboveground tanks, and lack of geological storage hydrogen storage options in India.

5.3.4 Technology costs and performance assumptions

Techno-economic costs for hydrogen and ammonia cost assumptions are listed in Table 5.2. Techno-economic costs for electricity generation technologies in India are listed in Table 5.3. In general, these costs are relatively similar to the literature, besides the key costs outlined in the three transition speed scenarios (i.e., solar PV, onshore wind, electrolysers, and batteries). Fuel cost assumptions are listed in Table 5.4. LNG costs remain at historical levels, while coal, biomass, and domestic natural gas remain at low costs. Biomass and domestic natural gas are limited by availability, as highlighted in the subsequent section.

Table 5.2: Hydrogen and Ammonia Cost Assumptions (Production, Storage, Transport)

	2020	2030	2040	2050	Unit	Reference
Electrolyser						
CAPEX - Historical Mix	953	670	566	504	USD/kW	Way et al. [137]
CAPEX - Slow transition	939	543	274	178	USD/kW	Way et al. [137]
CAPEX - Fast transition	907	383	155	123	USD/kW	Way et al. [137]
O&M	1.5%	1.5%	1.5%	1.5%	of CAPEX	IEA [24]
Lifetime	25	25	25	25	years	IEA [24]
Efficiency	65%	72%	75%	75%	LHV of H2	
Ammonia Synthesis (HB + ASU)						
CAPEX (all scenarios)	4,500	4,500	4,500	4,500	USD/kgNH3/hr	[80]
O&M	2%	2%	2%	2%	of CAPEX	[6]
Electricity consumption	0.72	0.72	0.72	0.72	MWh/t NH_3	[6]
Lifetime	30	30	30	30	years	[6]
Ammonia Storage						
CAPEX (all scenarios)	0.56	0.56	0.56	0.56	USD/kgNH3	[203] [204]
O&M	3%	3%	3%	3%	of CAPEX	[204]
Lifetime	30	30	30	30	years	[204]
Hydrogen Storage (aboveground)						
CAPEX (all scenarios)	689	572	378	345		DEA [144]
O&M	3%	3%	3%	3%	of CAPEX	[204]
Lifetime	30	30	30	30	years	DEA [144]
Hydrogen Pipeline						
CAPEX	940,000	940,000	940,000	940,000	USD/GW-km (LHV of H2)	IEA [24]
Lifetime	40	40	40	40	years	IEA [24]
Ammonia pipeline						
CAPEX	690,000	690,000	690,000	690,000	USD/GW-km (LHV of NH3)	IEA [24]
Lifetime	40	40	40	40	years	IEA [24]
Ammonia ship						
CAPEX	85	85	85	85	Million USD	IEA [24]
capacity	53,000	53,000	53,000	53,000	tNH3	IEA [24]
ship speed	30	30	30	30	km/hr	IEA [24]
Annual OPEX	4%	4%	4%	4%	of capex	IEA [24]
Fuel use	2,500	2,500	2,500	2,500	MJ/km	IEA [24]
Lifetime	30	30	30	30	years	IEA [24]

Table 5.3: Electricity Generation Technologies in India

	2020	2030	2040	2050	Unit	Reference
Utility-Scale Solar PV						
CAPEX - Historical Mix	626	470	380	320	USD/kW	[137][1]
CAPEX - Slow transition	626	380	240	160	USD/kW	[137][1]
CAPEX - Fast transition	626	270	140	100	USD/kW	[137][1]
O&M	9,800	7,900	6,700	6,000	USD/ MW/yr	DEA [87]
Lifetime	25	25	25	25	years	DEA [87]
Onshore wind						
CAPEX - Historical Mix	1,054	920	830	770	USD/kW	[137][1]
CAPEX - Slow transition	1,054	850	700	600	USD/kW	[137][1]
CAPEX - Fast transition	1,054	770	600	520	USD/kW	[137][1]
Fixed Costs	17,000	16,500	15,600	14,500	USD/ MW/yr	DEA [87]
Variable Costs	1.854	1.7613	1.6686	1.55	USD/MWh	DEA [87]
Lifetime	27	30	30	30	years	DEA [87]
4-hour grid scale battery						
CAPEX - Historical Mix	337	237	194	168	USD/kWh	Way et al. [137]
CAPEX - Slow transition	326	150	92	67	USD/kWh	Way et al. [137]
CAPEX - Fast transition	326	129	70	54	USD/kWh	Way et al. [137]
Fixed Costs	600	600	600	600	USD/ MW/yr	DEA [87]
Variable Costs	2.66	2.6	2.13	1.6	USD/MWh	DEA [87]
Roundtrip Efficiency	86%	86%	90%	95%	%	DEA [87]
Lifetime	20	20	20	20	years	DEA [87]
CCGT (NG or NH3 fuelled)						
CAPEX	776	776	776	776	USD/kW	[205][2]
Fuel Efficiency	60%	60%	60%	60%	% of LHV of fuel	[205][2]
Fixed Costs	17,353	17,353	17,353	17,353	USD/ MW/yr	[205][2]
Variable Costs	5	5	5	5	USD/MWh	[205][2]
Lifetime	30	30	30	30	years	[205][2]
OCGT (NG or NH3 fuelled)						
CAPEX	770	730	700	680	USD/kW	[206]
Fuel Efficiency	34%	36%	38%	40%	% of LHV of fuel	[206]
Fixed Costs	23,200	23,200	23,200	23,200	USD/ MW/yr	[206]
Lifetime	25	25	25	25	years	[206]
Biomass power plant						
CAPEX	950	950	950	950	USD/kW	CERC [207]
Fuel Efficiency	31%	31%	31%	31%	% of LHV of fuel	CERC [207]
Fixed Costs	58,480	58,480	58,480	58,480	USD/ MW/yr	CERC [207]
Lifetime	30	30	30	30	years	CERC [207]
Nuclear Power Plant						
CAPEX	2800	2800	2800	2800	USD/kW	IEA [180]
Fuel Efficiency	33%	33%	33%	33%	% of LHV of fuel	EIA [208]
Fixed Costs	100,000	100,000	100,000	100,000	USD/ MW/yr	EIA [208]
Lifetime	50	50	50	50	years	EIA [208]
Hydro Reservoir						
CAPEX	1,460	1,460	1,460	1,460	USD/kW	CERC [207]
Fixed Costs	37,000	37,000	37,000	37,000	USD/ MW/yr	CERC [207]
Lifetime	50	50	50	50	years	
Hydro Small						
CAPEX	1,023	1,023	1,023	1,023	USD/kW	CERC [207]
Fixed Costs	41,000	41,000	41,000	41,000	USD/ MW/yr	CERC [207]
Lifetime	35	35	35	35	years	
Hydro Run-of-River						
CAPEX	1,460	1,460	1,460	1,460	USD/kW	CERC [207]
Fixed Costs	37,000	37,000	37,000	37,000	USD/ MW/yr	CERC [207]
Lifetime	50	50	50	50	years	
Pumped storage						
CAPEX	860	860	860	860	USD/kW	[206]
Fixed Costs	8,000	8,000	8,000	8,000	USD/ MW/yr	[206]
Variable Costs	1.3	1.3	1.3	1.3	USD/MWh	[206]
Lifetime	50	50	50	50	years	[206]
Coal sub critical						
CAPEX	1,650	N/A	N/A	N/A	USD/kW	[206]
Fuel Efficiency	34%	N/A	N/A	N/A	% of LHV of fuel	[206]
Fixed Costs	45,300	N/A	N/A	N/A	USD/ MW/yr	[206]
Variable Costs	0.13	N/A	N/A	N/A	USD/MWh	[206]
Lifetime	30	N/A	N/A	N/A	years	[206]
Coal super critical						
CAPEX	1,400	N/A	N/A	N/A	USD/kW	[206]
Fuel Efficiency	37%	N/A	N/A	N/A	% of LHV of fuel	[206]
Fixed Costs	41,200	N/A	N/A	N/A	USD/ MW/yr	[206]
Variable Costs	0.12	N/A	N/A	N/A	USD/MWh	[206]
Lifetime	30	N/A	N/A	N/A	years	[206]

[1] Based on Way et al. [137], adapted to India using IRENA [136] historical global percentile. [2] NG based costs from Uniper and UK BEIS [205]

Table 5.4: Fuel Prices in India

	2020	2030	2040	2050	Unit	Reference
Domestic NG	5.78	5.78	5.78	5.78	USD/GJ (LHV)	[209][1]
Imported LNG	12.6	12.6	12.6	12.6	USD/GJ (LHV)	[209][2]
Coal	2.63	2.97	3.04	3.04	USD/GJ (LHV)	[210][3]
Nuclear	2.78	2.78	2.78	2.78	USD/GJ (LHV)	[180][4]
Biomass	4.42	4.83	5.34	5.9	USD/GJ (LHV)	[207][5]

[1] 4-5.5 USD/MMBTU (HHV) from Ministry of Power [209] [2] 10-12 USD/MMBTU (HHV) from Ministry of Power [209] [3] 3 USD/MMBTU [210] [4] IEA [180] [5] CERC [207] with 1%/yr escalation

5.3.5 Technology availability

Natural Gas:

Domestic natural gas reserves are limited in India, with historical performance far below expectations. The IEA assumes domestic production will make a turnaround and increase from 31 billion cubic meters (bcm) in 2020 to 66-101 bcm by 2040 [68]. Today, these domestic reserves are allocated by the government between the fertiliser, city gas, power, refining, and other sectors, with the power sector only getting roughly 25%, or 7.5 bcm, of this domestic gas [68]. The forecasts for increasing production in India are repeatedly missed. In 2019, the Ministry of Petroleum & Natural Gas "assured" (sic) a governmental committee that domestic production would significantly increase to 60.5 bcm production in 2021-2022 [209], and yet it still remains below 30 bcm in FY2021. In this thesis, it was assumed that production is increased to 66 bcm by 2040 in line with the IEA SDS scenario [68] and 25% of this domestic gas would be available at 5.5 USD/MMBTU.

Hydropower and biomass:

Total hydro power potential is estimated at 145 GW, with 41 GW installed and in operation [211]. Regarding hydropower, the government recognises that while full development of the potential is technically feasible, it faces serious environmental and social concerns [201]. The full potential was available, but not utilised in the results due to costs. Biomass potential is estimated at 25 GW in India and specified by region in [201].

CCS:

CCS technologies were not considered in either hydrogen production (i.e., blue hydrogen) or post combustion CCS for coal or gas fired power generation. Currently, the technical potential and costs for developing CO_2 storage in India is highly uncertain [2]. The potential locations are small and disparate, with diverse geology, and thus many of them would need to be exploited at a high aggregate cost for a single significant CCS project [2]. Further justification for ignoring CCS potential in India is that India's low quantity of domestic natural gas and high price of imported LNG makes natural gas with CCS unlikely to be cost competitive with green hydrogen or other forms of dispatchable electricity (e.g. ammonia GTs. Finally, India's targets as part of the NHM are focused on only *green* hydrogen and ammonia [18], further emphasising that "blue" technologies are not politically relevant in the Indian context.

Fossil fuel power generation:

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 [180].

5.3.6 Electricity Demand

Country wide demand projections: The basis for the electricity demand scenario is TERI's low-carbon scenario from [2], which increases to 6,200 TWh (excluding electricity for green ammonia for shipping, which TERI did not include) by 2050, as shown in Figure 5.6a and Table A.3. The electricity demand is forecasted using underlying economic scenarios based on OECD projections (note: before COVID), and growth in the sectors of residential, commercial, transport, industry, agriculture, and hydrogen as shown in Figure 5.6a and Table 5.1. In TERI's low-carbon scenario, compared to TERI's baseline scenario, more EVs and more electrolysis increase electricity demand over the baseline scenario, while increasing electricity efficiency measures decrease demand; however, the net effect is an increase in electricity demand from 5,300 TWh to 6,200 TWh in 2050. This demand forecast is largely in agreement with IEA demand forecasts up to 2040, as seen in Figure 5.6b.

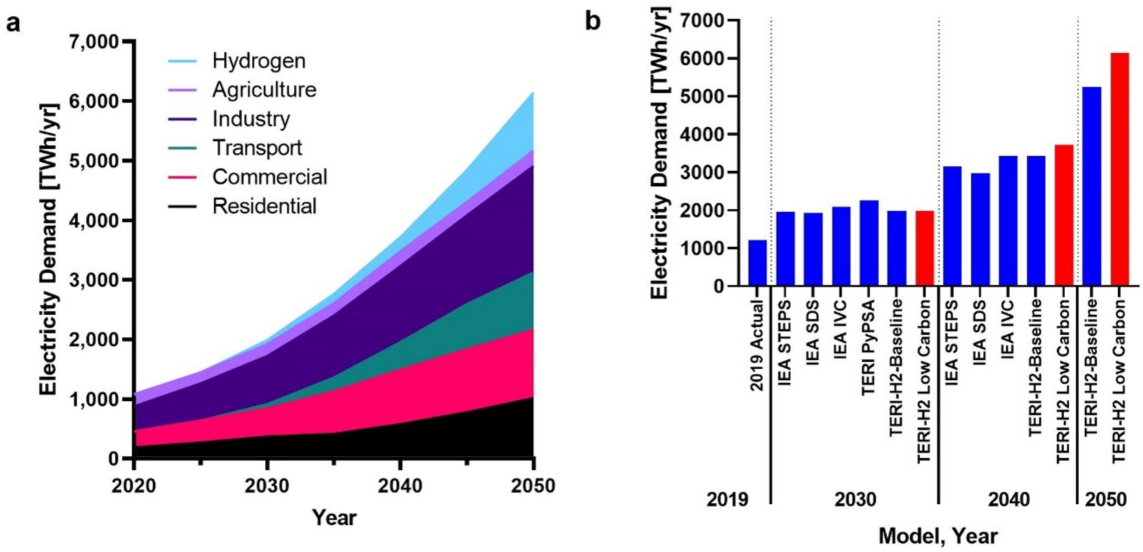


Figure 5.6: a. Electricity demand by major end-use sector, from TERI [2], enumerated in Table 5.1. b. Comparison of the electricity demand used in this study (red) from TERI [2] with demand forecasts from the IEA in different scenarios (blue) and TERI's baseline (blue).

Monthly and hourly electricity demand profiles:

The total electricity demand is split into regional demands based on historical splits from [202], with 90% of the electricity demand occurring in the NR, WR, and SR, as shown in Figure 5.7a and Table 5.1. The split is kept constant to 2050. The monthly and hourly demand data is generated from published reports from the Power System Operation Corporation Ltd. (POSOCO) for a typical day from each month in specific states [212]. States in the same regions are averaged to create the regional hourly demand for each day in each month of the year. Figure 5.7b shows the monthly output variation by region, and Figure 5.7c shows the daily profile used in each region in 3 months of the year. These demand profile shapes are kept constant to 2050, while the absolute level is increased with the increasing electricity demand of Figure 5.6a.

No demand side response in cooling or heating (i.e., thermal sector coupling), or smart charging of EVs are included in the model. The limitations of this assumption are discussed in subsequent sections.

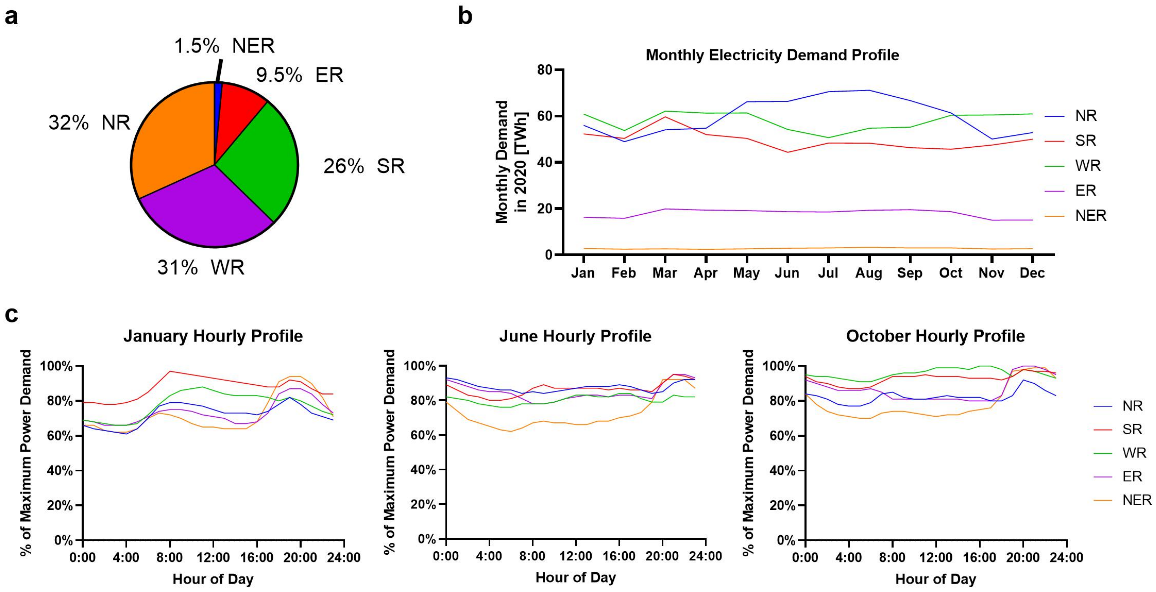


Figure 5.7: a. Electricity demand split by region, b. Electricity demand by region over months, c. Electricity demand by region for a daily profile in January, June, and October.

5.3.7 Hydrogen and Ammonia Demand Profiles

Demand for hydrogen and ammonia for the sectors of steel, fertiliser, oil refining, transport, and shipping fuel were considered to be split evenly between the NR, SR, WR, and ER. Every hour of the year was assumed to require a steady demand of hydrogen or ammonia. In some sectors, this is justified. For example, road transport (i.e., H_2-powered heavy duty vehicles) and shipping demand are likely to be relatively flat throughout the year. Steel demand is also likely to be relatively flat, unless H_2 DRI-EAF based steel production is technically able to operate flexibly, which is not clear at this point. Therefore, a flat demand is a more conservative estimate.

Fertiliser demand would be expected to follow the growing seasons of Kharif (Apr - Sep) and Rabi (Oct – Mar).[1] Nitrogenous fertiliser sales data (urea) from the Ministry of Fertilizers [19] is shown by state in Figure 5.8a for the ten largest consuming states, and with total country aggregated urea sales shown in Figure 5.8b. The dispatch of domestic and imported urea is shown in Figure 5.8b, from [19], which is relatively flat throughout the year. It is not clear why there is a discrepancy between sales and dispatch. A flat hourly demand throughout the year was used as a conservative approach, but this is an area where further work should understand the variation in actual application of nitrogenous fertiliser throughout the year in different states.

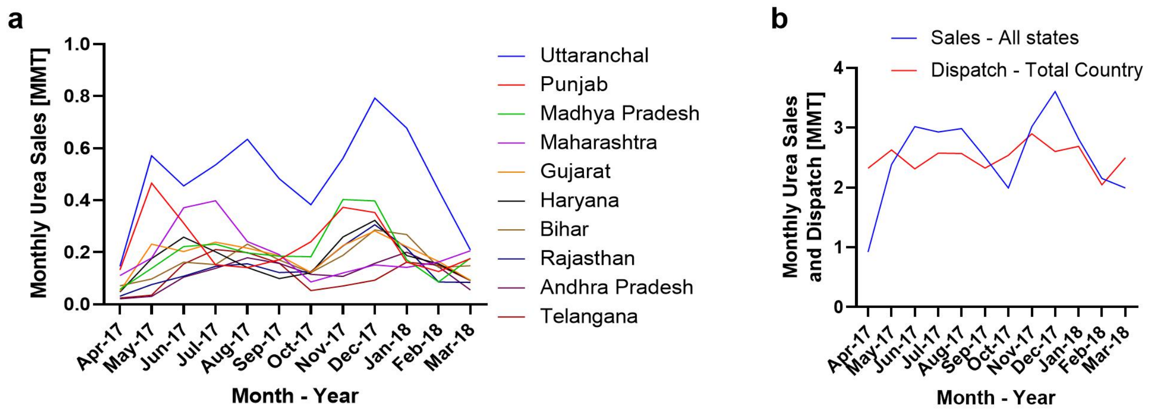


Figure 5.8: a. Nitrogenous fertiliser sales data (urea) from the Ministry of Fertilizers [19] by state for the ten largest consuming states over Kharif 2017 and Rabi 2017-18 growing seasons. b. Total country monthly aggregated urea sales and total country monthly urea dispatch (both domestic and imported) from the Ministry of Fertilizers [19].

[1] Kharif and Rabi mean *autumn* and *spring*, respectively, in Arabic. They are the names given to the main crop seasons in India, Pakistan, and Bangladesh. The Kharif crops include rice, maize, soybean, peanut, cotton, etc. and aligns with more rainfall during the monsoon (Apr - Sep). The Rabi crops include wheat, barley, oats, chickpeas, etc. and is the period of Oct - Mar [213]

5.4 Results

5.4.1 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 Levelised Cost of Hydrogen (LCOH) and Ammonia (LCOA) by 10% to 25% across the scenarios (Figure 5.9a, 5.9b, Table A.4). The reduction in LCOH and LCOA is driven by lower electricity prices available to grid connected electrolysers because they gain access to electricity that would otherwise be curtailed. In the islanded production scenarios, 15% to 20% of electricity generated in India in 2050 is curtailed, while only 10% to 14% is curtailed in the grid connected scenarios (Figure 5.9c, Table A.5). 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 electrolysers to the grid reduces annual system costs by approximately 5% in 2050 across all scenarios (Figure 5.9d, Table A.6). Beyond reducing costs, benefits of grid connected electrolysers include reducing material consumption and land-use associated with the extra solar PV that is no longer required.

Grid connected electrolysers and ammonia synthesis plants are operated seasonally to access cheaper, otherwise curtailed electricity, with significant ammonia storage to manage seasonal and interannual variations (Figure 5.10). Across all scenarios, ammonia production mostly occurs from March until August, with plants' loads reduced to minimum technical levels outside of these months (Figure 5.10a). These months correspond to the strongest solar resource in the Northern Region, and strongest wind resource in the Western and Southern Regions due

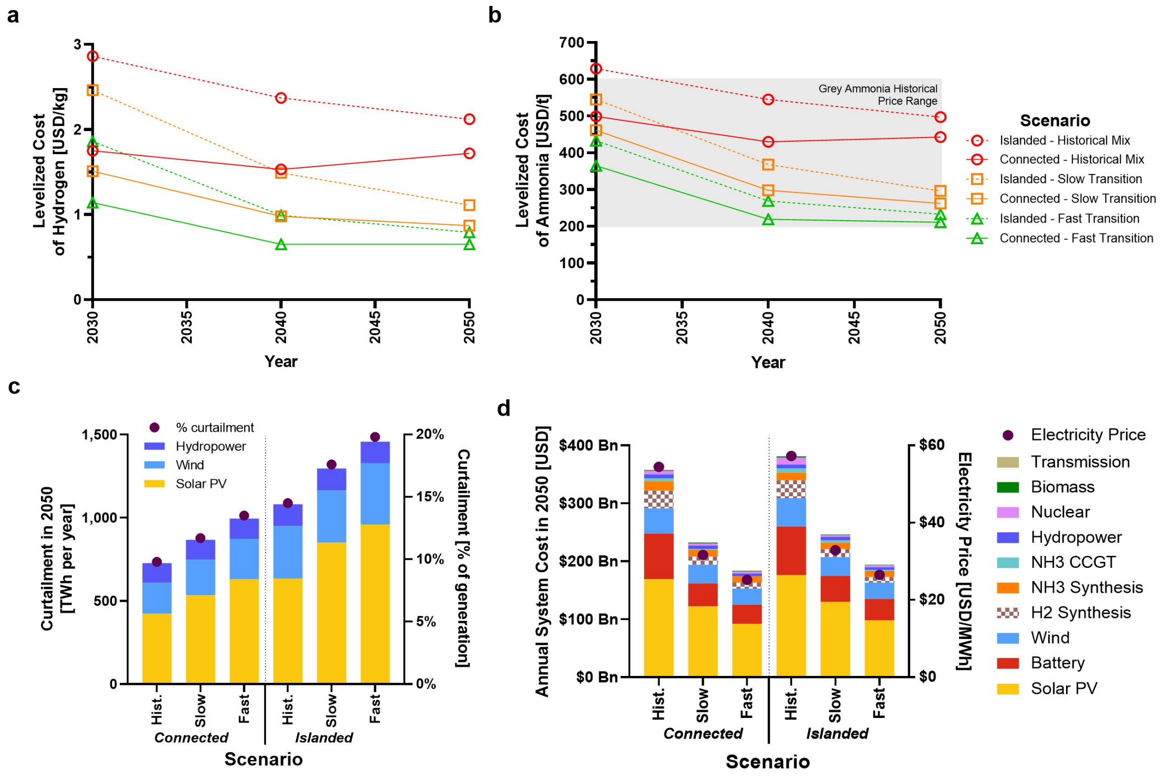


Figure 5.9: Key result metrics across grid connected and islanded system scenarios. a. LCOH across scenarios from 2030-2050 (see Table A.4), b. LCOA across scenarios from 2030-2050 (see Table A.4) with grey ammonia historical commodity price (Black Sea) from [20], c. Curtailment across scenarios in 2050 (further detail in Table A.5), d. Annualized system costs across scenarios in 2050 (further detail in Table A.6)

to the monsoon. Ammonia storage is required for the system to maintain a constant output of ammonia for fertiliser and shipping demand, ranging from 15 to 40 MMT of ammonia storage (Figure 5.10b). Simulating the 2050 system with weather data from ten consecutive Weather Years (WY1-WY10, corresponding to 2010-2019), the system's storage levels are nearly emptied in January and reach their maximum in August. The difference in Weather Year (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 5.10b).

The Historical Mix cost scenario requires more ammonia storage capacity (40 MMT) than the Slow (25 MMT) or Fast (15 MMT) scenarios. This result occurs because solar PV and wind are relatively more expensive in the Historical Mix scenario, and thus the optimisation finds that it is lower cost to buffer ammonia rather than overbuild solar and wind, which is the lower cost method for meeting seasonal demand in the Slow and Fast scenarios. This effect can also be observed in higher levels of curtailment in the Slow and Fast scenarios than the Historical Mix scenario (see Figure 5.9c). 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 utilised ammonia or hydrogen trading between regions via pipeline, truck, or ship for industrial demands (i.e., steel, fertiliser, transport, refining, maritime fuel). The ammonia production cost difference between regions was less than 50 USD/t, which is a relatively small difference, and justifies regional production. Instead of moving energy-storing molecules, the results point towards moving electricity via an increase in grid connected transmission lines (Figure 5.13c and Table A.10).

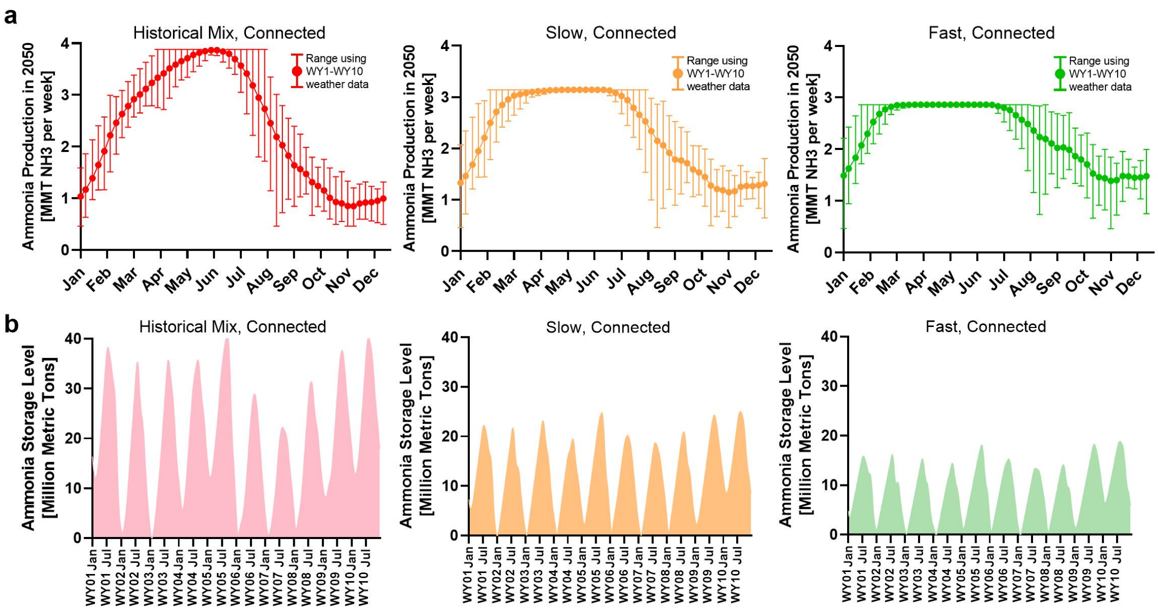


Figure 5.10: Seasonal and interannual variation in ammonia production and storage levels to meet a constant demand. a. Country-wide weekly ammonia production in 2050 across Connected scenarios, showing the range of weekly ammonia production depending on year of solar and wind data, b. Country-wide storage levels of ammonia in 2050 over 10 weather years (WY1-WY10) of solar and wind data in simulation.

5.4.2 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 5.11a). 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, Connected scenario to provide seasonal storage and resilience to unfavourable 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 utilisation factor of 2% to 5%, far lower than current power-plant utilisation factors.

In the Islanded scenarios, ammonia is used for seasonal power generation and system resilience in the Oct-Jan period (Figure 5.11b). In the Connected scenarios, the requirement for seasonal dispatchable electricity is notably reduced due to sector coupling effects. As shown in Figure 5.11b, WY1 and WY5 required the most dispatchable electricity via ammonia-to-power for providing system resilience. The amount of ammonia used in the power sector for generating power varies from 0 to 9 MMTPA as shown in Figure 5.12.

5.4.3 Decarbonisation results

The evolution of the Indian power system depicted across our scenarios is dominated by solar power with battery storage (Figure 5.13a, Table A.8). Across scenarios, solar PV installed capacity reaches over 4,000 GW by 2050, with 1,000 GW of 4-hour battery storage (see Table A.8). The installed capacity is concentrated in the Northern Region (NR), Western Region (WR), and Southern Region (SR) (Figure 5.14). Onshore wind power is mostly installed in

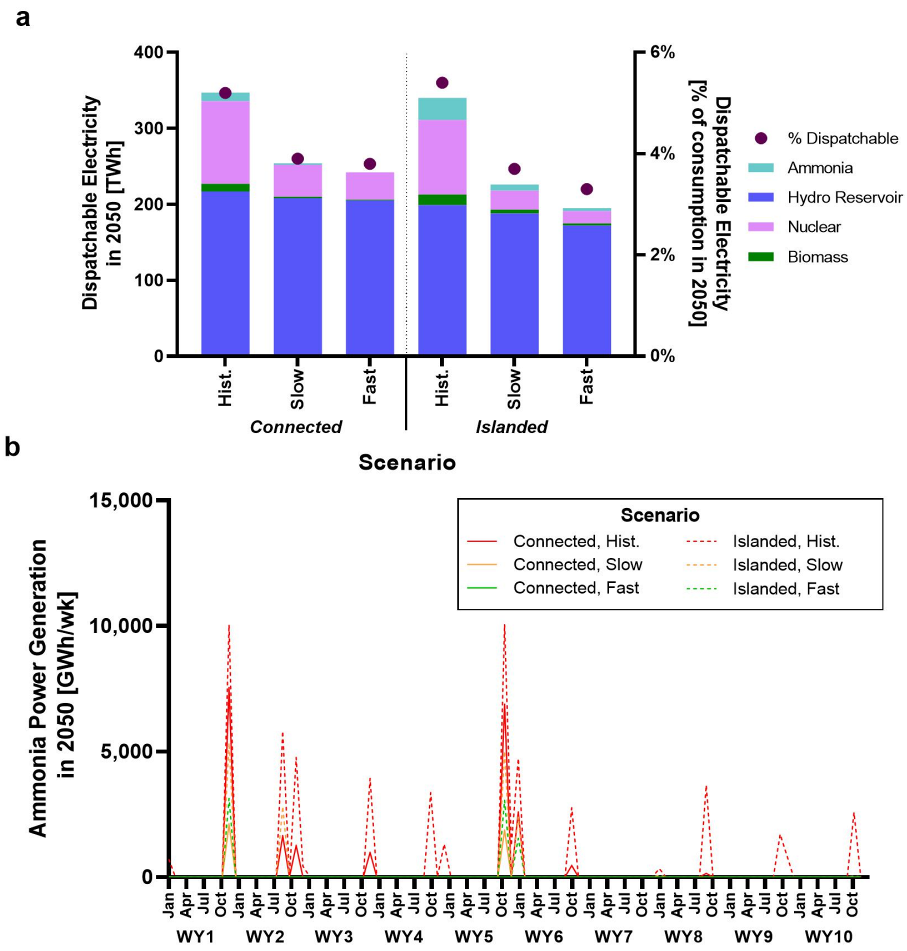


Figure 5.11: Dispatchable electricity requirements; a. Country-wide annual electricity generated from dispatchable assets in 2050 across scenarios, and relative percentage of total electricity consumed, b. Country-wide weekly ammonia GT power generation in 2050 over 10 simulated weather years (WY1-WY10) of solar and wind data.

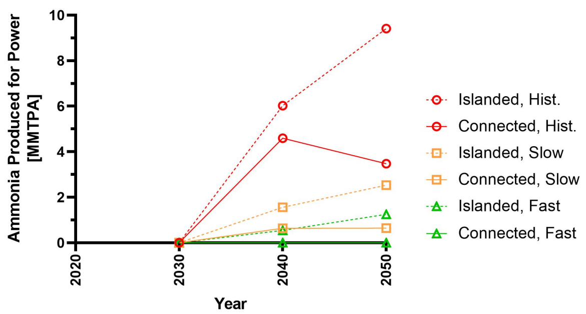


Figure 5.12: Ammonia which is re-electrified via CCGT (i.e. ammonia-to-power) across the six scenarios

the WR and SR, totalling 330 GW to 460 GW in the country by 2050. Electrolyser 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 5.13c and Table A.10).

Electricity generation rapidly shifts towards wind and solar, and increasingly to solar over time (Figure 5.13b, Table A.9). Carbon emissions begin rapidly declining to near-zero by 2040 and zero by 2050 across all scenarios (Figure 5.13d), 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. 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.

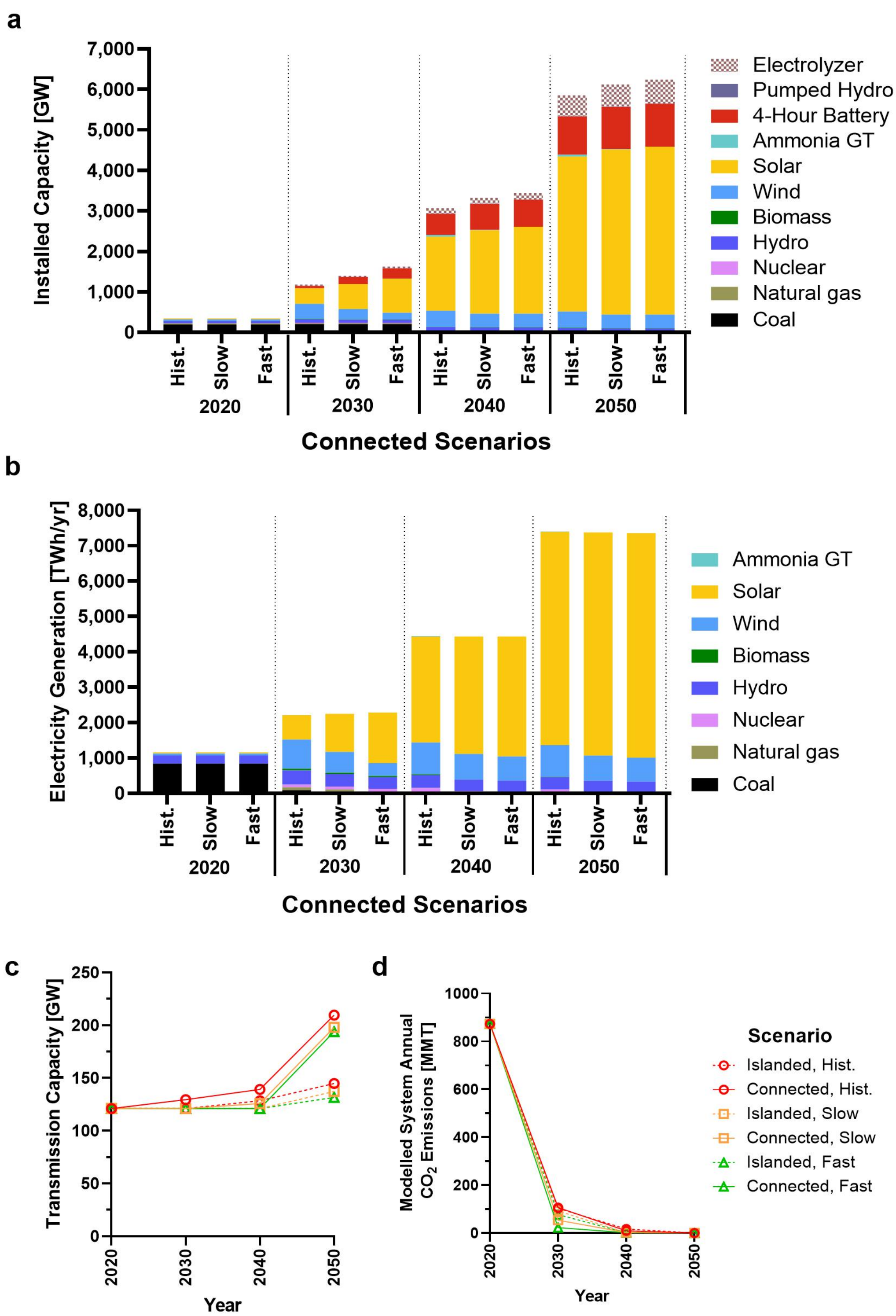


Figure 5.13: a. Installed capacity by year in the Connected scenarios, including grid connected electrolysers, with further data for Islanded scenarios in Table A.8. b. Electricity generation by year in the Connected scenarios, with further data for Islanded scenarios in Table A.9. c. Installed transmission capacity by year, also in Table A.10. d. CO_2 emissions from modelled system from 2020-2050, excluding emissions from non-electrified sources.

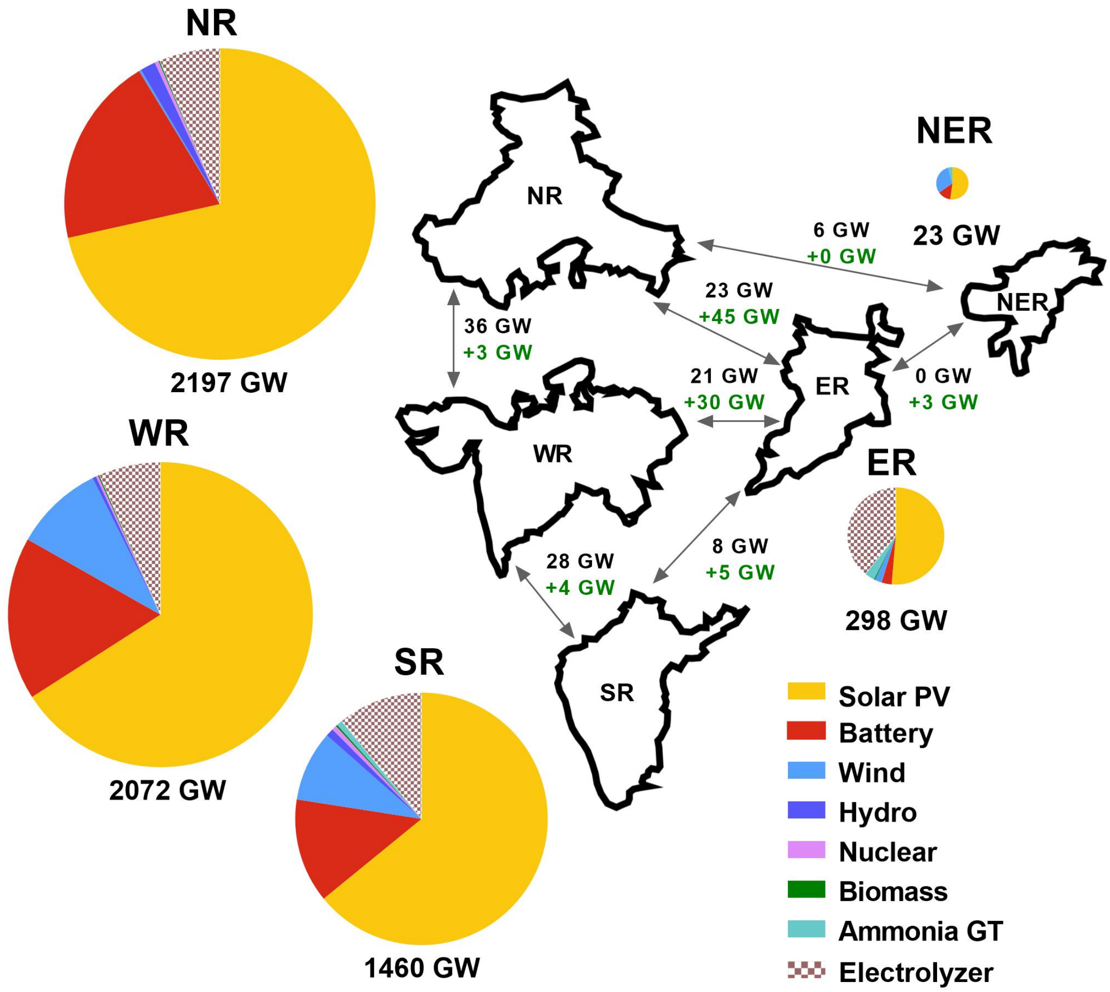


Figure 5.14: Generation capacity, battery capacity, electrolyser capacity, and transmission (new transmission in green) by region in the Slow, Connected scenario in 2050.

6 | Discussion

This chapter discusses the main findings from the thesis and highlights areas for improvements.

This chapter is segmented into four main sections: i) a discussion of the economic and geopolitical implications of the LCOH and LCOA results, ii) a discussion on the role of ammonia-to-power re-electrification, iii) a discussion of the role of green hydrogen and ammonia sector coupling, and iv) areas for improving the ESM modelling.

6.1 The new price of oil? Understanding LCOA and LCOH

LCOH and LCOA are useful key metrics for understanding the roles that hydrogen and ammonia may have in future decarbonised energy systems, and some of the key results of this thesis are (i) the LCOA found using the GSAM methodology for a widely achievable solar radiation location, and (ii) the country-wide LCOH and LCOA for producing hydrogen and ammonia at a national scale in India using a limited amount of VRE. From an economic perspective, LCOH and LCOA indicate when business models become viable versus alternatives, or at what CO_2 cost the incumbent fossil fuel technologies would become less competitive. Like the price of oil or natural gas, these green fuel cost forecasts can underpin rippling effects across the entire economy, and so the estimation of LCOH and LCOA must continue to improve from the wide-ranging values seen today via improved methodologies. In addition to economics, LCOH and LCOA have geopolitical implications as well which are discussed in this section.

6.1.1 Economic consideration of results

From an economics perspective, the LCOA in the islanded GSAM model outlined in Chapter 2 finds LCOA for 2020 to 2040 in a range that matches well with the more detailed modelling of the ESM of India from 2030 to 2050 across the six scenarios, as shown in Figure 6.1. Given the current momentum building towards decarbonisation and net-zero targets, reality is heading most closely in the direction of the Slow transition scenario used in the modelling. While India follows a relatively fast transition in the modelling in this ESM regardless of the price scenario, the Historical Mix, Slow, and Fast scenarios are median cost forecasts from a *global* transition scenario perspective. It is unlikely that the Historical Mix scenario will come to pass, and indeed if it did, it may cause significant environmental, health, and economic damages by 2050 that the other parts of the modelling, such as electricity demand, would need to be adjusted. Nevertheless, the Historical Mix scenario is useful as a comparison to more traditionally modelled component costs, such as those from the IEA, which fall between the Historical Mix and Slow scenarios, as shown in Figure 4.3.

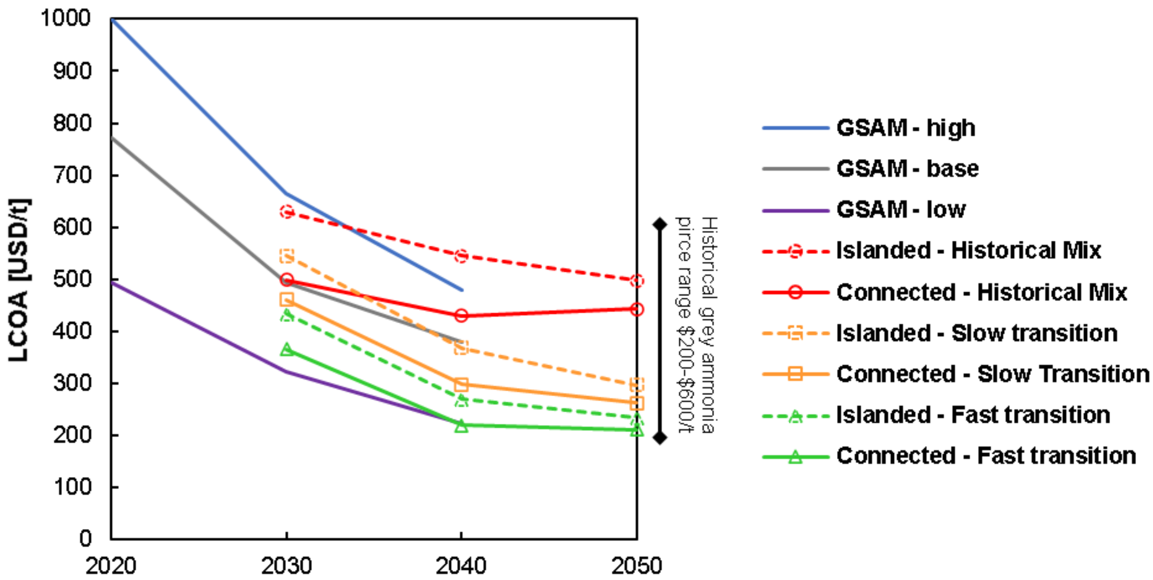


Figure 6.1: Combined LCOA results from the standalone modelling (GSAM) from Chapter 2 and the sector coupled ESM results in Chapter 4.

Compared with literature values, the LCOA results are generally significantly below the mainstream reports and in the same range as the few LCOA models which have similar component cost declines. Many of the mainstream shipping and international agency reports have far more pessimistic LCOA forecasts, such as Lloyd's Register [29] forecasting 350 to 400 USD/t in 2050 in the best locations, compared to this thesis's 200 to 300 USD/t in India (Figure 5.9b). The discrepancies can be traced to component costs, such as the electrolyser which Lloyd's Register assumes has a CAPEX of over 600 USD/kW in 2050, while the Historical Mix, Slow, and Fast costs are 504, 178, and 123 USD/kW, respectively (Table 5.2). Similarly, Fasihi et al. [77] forecast a range of 400 to 490 USD/t in 2030 and 310 to 380 USD/t in 2050, with electrolyser CAPEX only reducing to 270 USD/kW by 2050. On the other hand, there are other LCOA models in the literature which use similar ranges of component costs as this thesis. Nayak-Luke & Bañares-Alcántara find a range of 310 to 350 USD/t in the best locations by 2030, using an electrolyser CAPEX of 341 USD/kW in 2030 [6], which matches the Fast transition costs of this thesis. The risks of using estimates not based on learning curve analysis is pessimistic estimates for LCOH and LCOA which create a narrative that the transition to green alternatives will be very expensive. This narrative creates more barriers for actors to move today towards decarbonisation, while the learning-by-doing evidence suggests that the transition to green ammonia and hydrogen will indeed be cheaper with decisive action.

The LCOH and LCOA results from the India ESM suggest that green hydrogen and ammonia will be cheaper than incumbent fossil fuel technologies in several large sectors, notably steel and fertiliser production, by 2030. TERI found that below 2 USD/kg, green hydrogen used in steel production can compete with traditional fossil routes [2], and Indian industry leader Reliance has announced a target of 2 USD/kg by 2030 [214]. The LCOH in the Indian ESM are below 2 USD/kg in all three connected scenarios by 2030 and reach as low as 0.80

USD/kg in 2050 (Figure 5.9a). Similarly, the brown ammonia production cost for fertiliser in India is estimated at 330 to 520 USD/t based on 7 and 11 USD/mmBTU natural gas, respectively [2], while this thesis's model finds the Fast and Slow scenarios can compete already in 2030 with LCOA between 365 to 545 USD/t (Figure 5.9b). Certainly in 2040 and 2050, the green route to ammonia production appears to be lower cost than gas-based ammonia, without any CO_2 price considerations. In summary, the LCOH and LCOA presented in this modelling gives reason for optimism. LCOH and LCOA at these levels are near cost competitiveness with fossil fuel alternatives, and well on the path towards becoming cheaper than fossil-fuel derived alternatives in key sectors like steel and fertiliser production.

6.1.2 Geopolitical considerations of results

Similar to oil and gas, hydrogen and ammonia are likely to cause geopolitical shifts as well. IRENA has recently published a report that investigates exactly this topic; "Geopolitics of the Energy Transformation: The Hydrogen Factor" [21]. Essentially, hydrogen and ammonia have the potential to (i) reduce geopolitical importance of some fossil fuel exporting nations, (ii) allow some fossil fuel nations to transition from exporting fossil fuels to exporting green fuels (e.g., Oman, Saudi Arabia, Australia) or blue fuels (e.g., Russia, Norway, Australia), (iii) allow for previous importers to become more energy independent (e.g. India, China, Chile, Morocco), and (iv) allow for new exporters to enter and diversify the market (e.g., Chile, Morocco and North African nations, Namibia and Southern Africa nations) [21]. Additionally, hydrogen and ammonia could result in relocation of heavy industries, such as steel, to places with lower cost hydrogen production for a green industrialisation [21]. For example, in India, steel is predominantly in the Eastern Region, close to coal resources, while a future may see new steel in the Southern, Western, and Northern Regions where VRE is lower cost and land is more available. However, there are many reasons for industries to remain where they are despite a VRE cost advantage of moving, such as the human capital, infrastructure, and labour costs [21].

Despite the excitement and attraction of shifting away from relying on the fossil fuel incumbents for energy, the fact remains that hydrogen and ammonia are not a like-for-like replacement for gas and oil, for at least three reasons. First, experts doubt that the quantities of hydrogen or ammonia (or methanol) will generate as much revenues as oil and gas do today, as shown in Figure 6.2. Secondly, the process of hydrogen and ammonia production is fundamentally a conversion process of VRE into chemicals, versus an extraction process of oil or gas which can fetch much higher profits for a nation [21]. Instead, the ownership of the intellectual property, such as the electrolysers, will be more important for extracting value [21]. The vast majority of patents in the hydrogen space are from Europe, USA, Japan, Republic of Korea, and China, with little contribution to date from India, Africa, the Middle East, or Latin America [21]. Thirdly, many players can enter the space with similar cost green hydrogen or ammonia based on similar VRE resources, while economically viable extraction of oil and gas are inherently much more concentrated in fewer nations, with over 80% of the world's population living in a fossil fuel importing country [21]. Therefore, one can imagine that as the hydrogen economy diverges from fossil fuels, the geopolitical influence of energy trade is reduced.

Ultimately, the LCOH, LCOA, and ESM findings from this thesis support three main ideas regarding the geopolitics of hydrogen and ammonia. First, the findings support the idea that the variation in LCOH and LCOA will be relatively small across regions and many nations will be able to produce hydrogen and ammonia at similar prices. This result is found in the GSAM, which uses a general solar profile available in many geographies, as well as in the ESM results in the different regions of India, in which the difference in LCOA is less than 50 USD/t, and

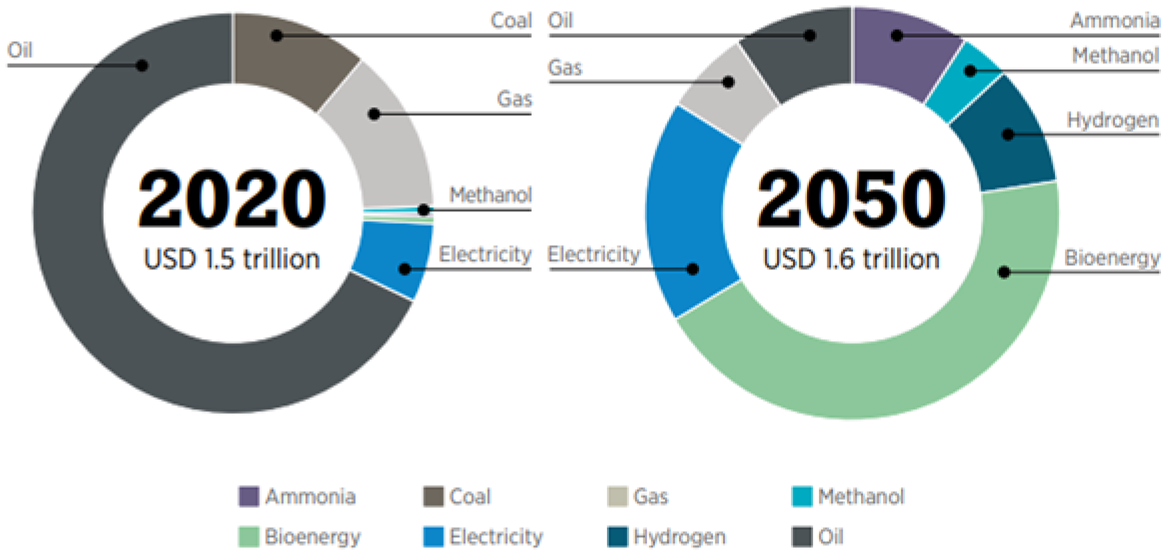


Figure 6.2: IRENA forecast of the value of trade in energy commodities, 2020 to 2050 [21].

thus less than building an ammonia trading infrastructure. The implication of this finding is that the market will not be dominated by a few actors like oil and gas. Additionally, in the Indian context, this finding gives some hope that a massive labour and industrial shift from the east to the west need not occur overnight. Instead, a grid connected system is optimally designed to locate production in all regions where there is demand and connect the regions with transmission because, in this modelling, it is more cost effective to trade electricity via transmission lines than to trade molecules.

Secondly, the findings support the idea that green hydrogen and ammonia can dramatically improve energy security and reduce imports. India's NHM explicitly states, "The implementation of this Policy will provide clean fuel to the common people of the country. This will reduce dependence on fossil fuel and also reduce crude oil imports" [18]. Indeed, the level of LCOH and LCOA achieved are more competitive than importing fossil fuels for the steel and fertiliser sectors in India. In fertiliser, India is effectively 80% reliant on imports for ammonia production today: 25-30% of India's consumption of fertiliser is imported ammonia and over 60% of the domestically produced ammonia is produced used imported LNG [68]. This reliance on imports is a major strategic reason for India to shift towards domestic green ammonia production for fertilisers and the results of this ESM suggest that this is possible in the near-term without a subsidy or a CO_2 pricing mechanism. Furthermore, other models, such as the IEA's India Energy Outlook STEPS scenario, forecast a tripling of the fossil fuel import bill in India to 2040 [68]. Oil is predominantly used in road transport, and there is huge oil demand growth forecasted by the IEA in trucks specifically [68]. As described in Chapter 4, the assumptions of FCEV in trucking is limited to only 1% and 27% of new truck sales in 2030 and 2050 respectively (see Figure 5.3)[2]. TERI's subsector model, which is used for this forecast alongside a qualitative analysis to generate an estimate of BEV and FCEV penetration, uses higher hydrogen prices at the refuelling stations than found in this modelling, at 3.70 USD/kg in 2030 and 2.20 USD/kg in 2050 [2]. A lower LCOH would help with faster adoption of FCEVs, especially in trucking where FCEVs are most competitive, and thus less oil imports for India. These findings of green hydrogen and ammonia enabling reduced imports across sectors are relevant for other countries; Chile currently imports about 65% of its energy needs, Morocco 91% and Namibia 74% [21], and Morocco is one of the largest importers of ammonia today [20].

Thirdly, the findings support the potential for India to use surplus VRE capacity on barren lands to produce fuels for export, such as bunkering fuel. Again India's NHM explicitly states, "The objective also is for our country to emerge as an export Hub for Green Hydrogen and Green Ammonia" [18]. The findings suggest that India can indeed produce sufficient low-cost ammonia from the VRE resources using land-use categorisation assumptions (outlined in Chapter 3) to meet the demand of bunker fuel (outlined in Chapter 4) which meets 10% of the global shipping fuel demand by 2050.

6.2 Should ammonia be re-electrified? Maybe

The results of this thesis suggest taking a nuanced view towards the role of ammonia-to-power in the electricity sector. One on hand, ammonia-to-power is more attractive than other comparable dispatchable electricity generation technologies, such as hydrogen GT, nuclear, and post-combustion CCS. On the other hand, the sector coupled ESM points towards other forms of flexibility, such as seasonal demand side load-shifting and increased regional transmission, as more optimal system solutions in the Indian context, with ammonia-to-power playing a minor role. In this section, these nuances are further explored.

6.2.1 Ammonia-to-power for seasonal storage and resilience

The results clearly show that ammonia-to-power is useful for seasonal power generation as well as providing resilience to interannual variation, as shown in Figure 5.11. Fundamentally, this is driven by the need for a dispatchable technology that is economically viable at low utilisation. Other modelling studies in the literature agree that there is a technology gap where characteristics of ammonia GTs would fit quite well. Bloomberg's New Energy Outlook [12] identified a "Technology X" needed in the power sector at a utilisation less than 25% to provide dispatchable generation. Similarly, the IEA gave a 15% utilisation estimate for peaking gas turbines in future energy systems [24]. In order to decarbonise the last 5% of the USA's power system to 2050, Cole et al. needed to deploy 500 GW of hydrogen-fired GT to provide dispatchable electricity, with capacity factors as low as 6% permitted in the modelling [106]. This thesis's ESM of India found similar results to these models which find an important role for using a low utilisation dispatchable technology, as ammonia gas turbines were used at utilisation rates of 2% to 5% in the ESM. Furthermore, the results of the standalone LCOE analysis of Chapter

2 showed that a lower utilisation rate (see Figure 3.11) would favour ammonia GT over nuclear and other technologies, which indeed did occur in the Indian ESM's optimisation.

6.2.2 Four factors which affect the role of ammonia-to-power

While the results highlight the usefulness of ammonia-to-power, they are less pronounced than expected. The "Fast, Connected" scenario does not require ammonia, and even the highest amount of ammonia usage in the "Historical Mix, Islanded" scenario only accounts for 29 TWh or 0.5% of annual demand. These results suggest that the role of ammonia-to-power is small, but there are context specific factors in the Indian system which lead to a small role. There are at least four factors which will likely affect the level of ammonia-to-power required in an electricity system.

The first factor is the need to import power due to resource availability of solar and wind, as well as the political or technical availability of biomass, nuclear, and CCS-based power. For example, ammonia-to-power is likely to play a large role in Japan, where land availability is low, offshore wind is more expensive due to deep waters, natural gas is imported at a high price making CCS-based power too expensive, and nuclear power is socially unacceptable. Indeed the first Request for Proposals (RFP) for imported low-carbon ammonia for re-electrification has been announced by a coal plant operator in Japan [86]. Similar factors may require ammonia for power import to Singapore, South Korea, and Germany. On the other hand, India has large surplus of very low cost solar PV in Rajasthan (Northern Region) and in Maharashtra (Western Region), as well as significant biomass and hydro potential, which all enable the system to be self-sufficient without any need to import ammonia for re-electrification. Thus, this first factor does not contribute to any ammonia-to-power use in India, but is a relevant factor for considering the role of ammonia-to-power on a global scale.

A second factor which affects the role of ammonia-to-power is the shape of the solar and wind profile mix, and particularly the penetration of wind. Wind power requires other technologies to match both its seasonality and to provide resilience during wind droughts. Severe multi-week wind droughts are likely to be challenging for electricity systems such as in the UK, where they are relatively infrequent but require a long-duration storage or dispatchable generation technology to mitigate. Ongoing research by the Royal Society and Professor Sir Chris Llewellyn Smith finds that 130 TWh of hydrogen storage in salt caverns is required in the UK system to manage the wind-dominated system over multiple decades of weather data and wind droughts and in the absence of energy imports [215]. The annual UK demand of Smith et al.'s system modelling is 570 TWh, and thus 23% of annual demand must be available in storage. This would amount to 25 MMT of ammonia if ammonia storage was used in place of hydrogen salt caverns. On the other hand, solar PV power is fundamentally reliable because the sun comes up every day, and even in cloudy weather some amount of electricity is generated. There is no risk of the system suffering weeks without the sun coming up. In the Indian ESM, solar PV generation reaches close to 90% of power generation with onshore wind making up the remaining 10% (small fractions are met by hydro, biomass, and nuclear). The amount of ammonia storage used for seasonal load shifting is between 15 and 40 MMT of ammonia across the scenarios by 2050 (Figure 5.10b). This is similar in absolute quantity to the hydrogen storage required for long-term storage required in the UK system modelled by Llewellyn Smith et al., yet is an order of magnitude less in relative terms (i.e., 1% to 3% of annual Indian electricity demand stored as ammonia versus 23% of UK annual electricity demand stored as hydrogen in salt caverns) since the annual Indian electricity demand is nearly 7,000 TWh. Ultimately, the relatively low use of long-term storage and dispatchable electricity in India is a result of a solar-dominated system which does not face major seasonality and resilience requirements.

Wind based systems, which tend to be more seasonal and more subject to resilience challenges, such as inter-annual variation and multi-week wind droughts, may find ammonia-to-power to be a far more deployed technology.

A third factor hitherto unconsidered in the hydrogen and ammonia literature is the availability of industrial flexibility. As highlighted in the results of this thesis, seasonal industrial flexibility on the demand side can greatly reduce the need for dispatchable electricity on the supply side. This is clearly shown in the difference between the amount of ammonia-to-power deployed in the Connected scenarios (0 to 11 TWh/yr) versus Islanded scenarios (4 to 29 TWh/yr). India is a country where the role of heavy industry is relatively certain, while in other countries, such as the UK, the future role of steel, fertiliser, and shipping fuel production is much less likely. Indeed, IRENA highlighted the potential that heavy industry moves to areas with cheapest renewables and materials [21]. However, there are also counteracting forces beyond the cheapest VRE to consider, such as the role of industry in creating jobs and political reasons to support specific industries (e.g., the “Make in India” campaign, or energy security reasons for manufacturing one’s own wind turbines). Importantly, this thesis highlights that having hydrogen-intensive, flexible industry in a nation might help the grid by reducing long-duration storage requirements. Thus, nations such as the UK which have large long-duration storage requirements might economically *benefit* from hydrogen-intensive industry reducing these requirements, even if the VRE resources are not as cheap as in other locations. This is a new factor for electricity system planners and government departments of industrial strategy to consider as an outcome of this thesis.

A fourth factor affecting the role of ammonia-to-power is depth of decarbonisation which a nation strives to achieve, and if the final tonnes of CO_2 from existing fossil fuel assets are worth the cost of ammonia-to-power infrastructure. These backup plants will, by definition, be used very little, and therefore their CO_2 emissions will be quite low in absolute terms. This can be seen in the Indian ESM results in Figure 5.13d, where the system is almost decarbonised in 2040, even though some gas plants are operating at low utilisation. Along these lines, Cole et al. find that decarbonising the last 10% to 20% of the USA's grid will be far more expensive than the first 80% to 90%, with CO_2 costs having to reach over 600 USD/t CO_2 to justify switching from gas peakers to hydrogen peakers for the final 5% decarbonisation [106]. It may be more cost effective for governments to reduce CO_2 in other sectors, at least in the medium term, rather than focusing on this final 5% of the power system. Additionally, other ESM research of the USA grid finds that it is cheaper to invest in Carbon Dioxide Removal (CDR) technologies like DAC (assumed to effectively cost 200 USD/t CO_2 in 2050 in the USA) to offset the gas peaker plant emissions than to use hydrogen peakers [216]. This finding might not be true in India, where gas prices are very high, but could be true in contexts where natural gas is very low cost. Despite the economic justification for leaving the last few percentages of the power sector's CO_2 emissions, countries such as the UK have made clear targets for a 100% decarbonised electricity grid by 2035, apparently without any room for compromise [217]. In such a case, technologies such as ammonia-to-power which are close to technical maturity may be required.

In summary, four factors which affect the potential role of power-to-ammonia are: i) the availability of VRE and other dispatchable technologies, ii) the solar and wind profiles, and particularly the penetration of wind, iii) the availability of demand side flexibility, especially seasonal load shifting, and iv) the imperative to reach 100% decarbonisation, and the cost of emissions offsets for the final percentages.

6.3 Sector coupling of ammonia

As the momentum builds with more societies transitioning towards net-zero, both IAMs and more temporally granular ESMs need to continue to expand their scenarios to enable explorations of new clean energy pathways available for deep decarbonisation. At a global level, IRENA forecasts that the production of green hydrogen and its derivatives will use 30% of the total electricity demand in 2050 [21], which closely matches the 25% estimate for the Indian energy system in this thesis. Therefore, despite the current literature's oversight, the role of sector coupled hydrogen and hydrogen derivatives, such as ammonia, is far too large and important to continue omitting from ESM. There is an urgency to modelling sector coupling of hydrogen and ammonia because it is increasingly clear that fleets of electrolysers will be deployed at considerable scale starting this decade and related policy decisions are being made today.

6.3.1 Benefits for the grid

In this thesis, it is found that connecting large fleets of electrolysers into the grid infrastructure and load-shifting the industrial production, specifically green ammonia production for fertilisers and shipping fuel, is a plausible strategy towards a lower cost, more efficient, and more reliable electricity grid. This 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 fertiliser and shipping sectors as well as to provide firm generating capacity via ammonia-to-power in gas turbines. Smaller quantities of green hydrogen are stored aboveground for intra-daily load shifting. Seasonal stockpiling of chemical energy is already done today in Europe for natural gas storage, with roughly 1,200 TWh of storage, or one-fifth of the total European natural gas demand [5]. Therefore, this type of system is realistic to envision, especially given the low costs of aboveground ammonia storage.

While there are many benefits to the grid in the connected scenarios, the islanded scenarios highlight the costs of keeping sectors decoupled, and indeed this decoupled pathway is the current recommendation from the IEA [68] and TERI [2]. If ammonia and hydrogen production is not grid connected, the system is more expensive, green hydrogen and ammonia are more expensive, and the system is less resilient, requiring more ammonia-to-power for dispatchable back-up power. Islanded scenarios need to use seasonal dispatchable power generation (i.e., supply-side flexibility) because they do not have the demand-side, load-shifting flexibility of grid connected electrolysers to manage seasonality of the renewable resources. The reason modellers see decoupled as a better solution is because they focus on the hydrogen generation cost and current grid connection charges, and miss sector coupling effects which benefit the wider system.

6.3.2 Policy implications

The government of India is one of many governments seeking to understand the roles of hydrogen and ammonia in the future energy system. Both the questions of grid connecting industry and the need for long-duration storage or system resilience are relevant to policymakers in India today. The government's think tank, Niti Aayog, highlighted the roles that ammonia *could* play in dispatchable power generation, but did not quantify that role via an ESM-based analysis [218]. while not explicitly modelling it yet, it is clearly an area of interest.

Unfortunately, the potential benefits on the Connected scenarios' sector coupled 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 [219]. 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, electrolyser 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 the findings of this thesis, 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 green hydrogen and ammonia production. One policy aims to reduce grid costs for green hydrogen and ammonia plants by waiving interstate transmission charges [18]. While this is a good first step, the incentives and coordination for flexible industrial production still need to be developed. The suitability of policy and market mechanisms needs to be explored today, at the initiation of this transformation, in order to progress towards a better, more integrated future scenario.

6.3.3 Other risks and opportunities not captured in the least-cost model

As highlighted in the ROA framework in Chapter 3, a least-cost optimisation model misses the multi-criteria decision-making which underpins reality. Therefore, it is important to highlight the risks and opportunities that the results of the ESM may include. Three criteria beyond cost are considered in this section: land-use, water-use, and labour. This is not an exhaustive list of risks and opportunities, but highlights implications beyond cost which require further interdisciplinary research. While it is out-of-scope for this work to resolve these risks and opportunities, it is a key part of the discussion of the results.

6.3.3.1 Land use

First, there are significant risks to changing land use in a decarbonised system. In India, the technical potential of solar and wind based on different land-use categorisation varies widely across models; however, this assumption is extremely relevant in deep decarbonisation scenarios. Specifically, solar PV annual generation potential in India is reported to be 1,300 TWh by the National Institute of Solar Energy (NISE) [220], 3,000 to 15,000 TWh by TERI [2], and 20,900 TWh by Lu et. al [126]. Similar variation of an order of magnitude occurs in onshore wind power estimates, ranging from the National Institute of Wind Energy (NIWE) 1,700 TWh [14], to 4,300 from TERI [2], to 22,000 from Lu et. al [126].

Given that the demand forecast for electricity demand in India in 2050 is approximately 5,000 - 7,000 TWh [2], the technical potential assumptions are crucial for the planning of the electricity system. The variation stems from land-use assumptions. Figure 6.3 shows the difference in available land for solar PV in India when only barren land is considered versus cropland, using data from [16]. To date, most of the solar PV in India has actually been installed on cropland which has been re-purposed for power generation [221]. Despite this current trend, in this thesis, barren and shrubland was used as a conservative estimate for the technical potential to have minimal land disruptions. As a result, most of the solar PV is installed in the northwest and western areas which have the most available land as shown in Figure 6.3.

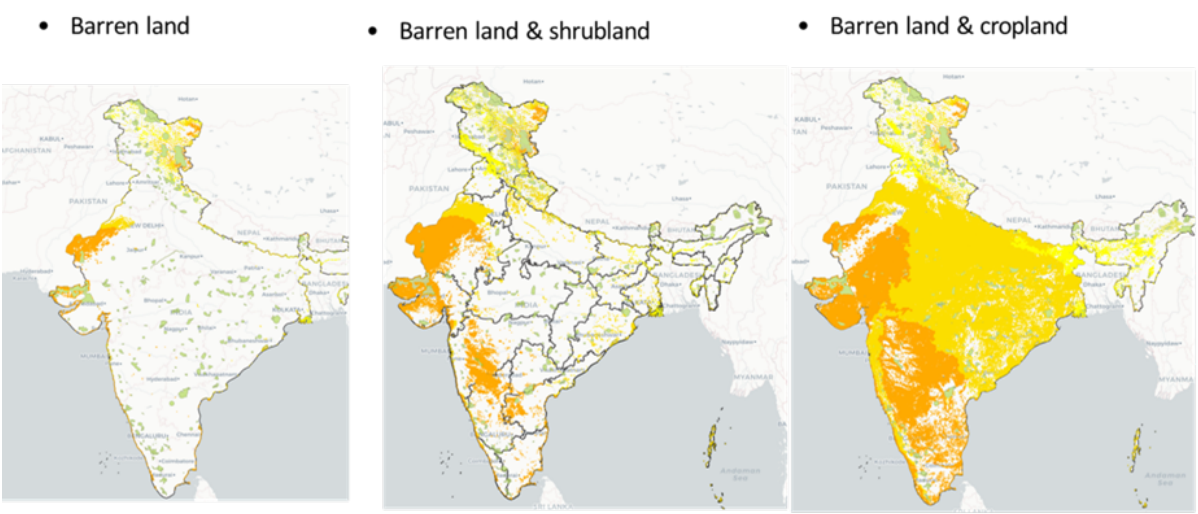


Figure 6.3: Different land availability assumptions for solar PV. Figures created and downloaded using NREL RED-E tool [16]. Yellow and orange indicates available land, with orange being of slightly better irradiance levels. Green areas are protected lands.

6.3.3.2 Water

A second major risk, and yet potentially also an opportunity is around water use. India is a very water stressed country, with 45% of its population facing acute water shortages [68]. Today, agriculture accounts for over 80% of water use in India, and there is clear evidence that water efficiency could be improved by severalfold in the agricultural sector of India [68]. Another large consumer of water in India is the power sector, which withdraws 30 billion cubic meters (bcm) of water and consumes 6 bcm of water in India, mostly at coal power plants and for bioenergy [68].

Green hydrogen uses pure water as a feedstock, and there are concerns for the water consumption, particularly as over 70% of announced electrolyser projects today are announced in water stressed regions which have favourable solar resources, e.g., Australia, Chile, Saudi Arabia, Oman, and Spain [21]. Assuming that each kilogram of green hydrogen requires 9 kg of water (stoichiometrically), then the 40 MMT of green hydrogen produced in this thesis's ESM by 2050 in India would require 0.4 bcm of water annually, or only 6% of the current

Indian power sector consumption. In short, electrolysis does not require very much water comparitively. This point is illustrated at a global scale in Figure 6.4, where IRENA's 2050 global hydrogen demand in a 1.5 C compatible scenario (including green and blue, even though blue requires more water than green), is two orders of magnitude smaller than the agricultural water demand [21]. Furthermore, since solar and wind power use less water for operation than thermal generation plants, it is estimated that India's power sector will reduce its water consumption by 84% by 2030 [21]. In summary, the risk of increasing water consumption via a shift to renewables and green hydrogen is very low. Indeed, there might be savings in the short-term in the switch from coal to solar PV and wind, while the long term may return to today's power sector levels due to the fourfold increase in demand for electricity to 2050.

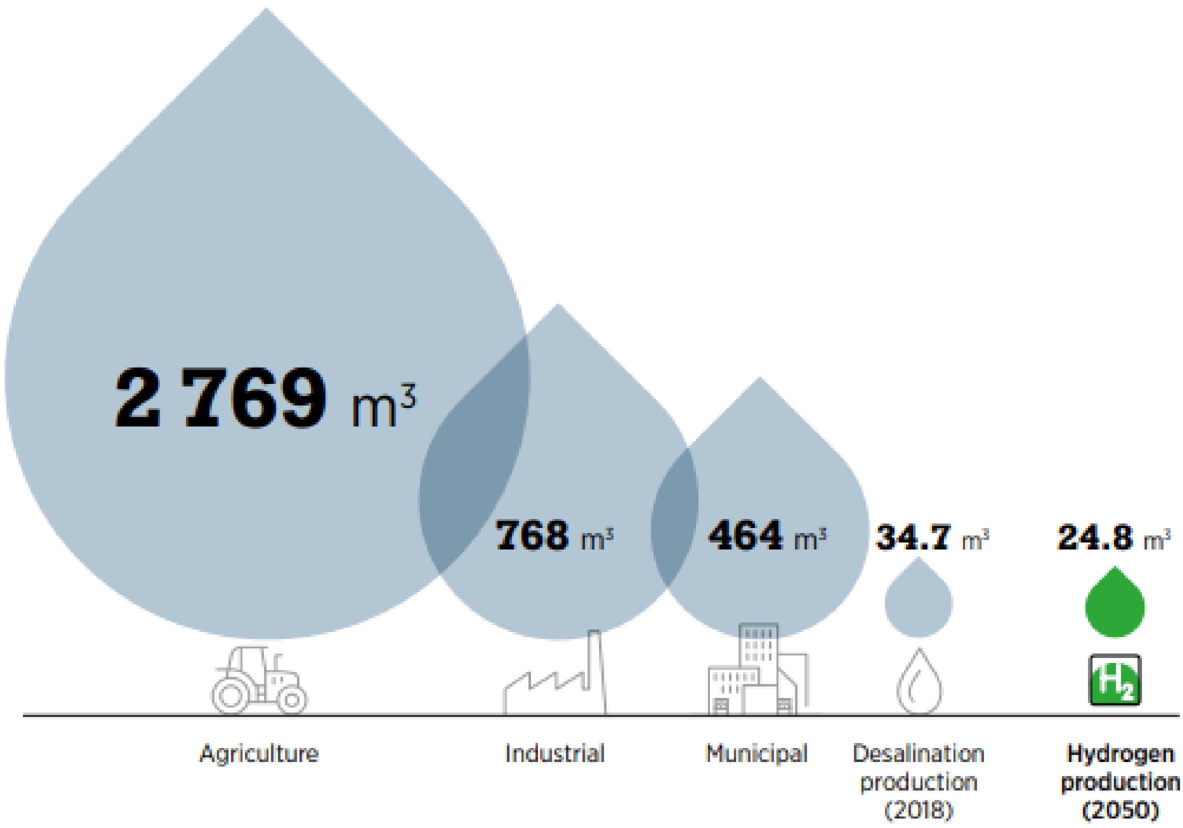


Figure 6.4: Global water consumption of hydrogen in 2050 in IRENA's 1.5 C scenario, compared with selected sectors today (billion cubic metres). Note that this figure is water consumption not withdrawals (i.e. it does not include water that is directly returned to the body it is taken from). Taken from IRENA [21].

While the risks of added water stress from green hydrogen can clearly be managed, there is actually an opportunity to use green hydrogen production to *improve* water security by building out desalination infrastructure which is either oversized or can be repurposed during times of water stress. Over 85% of announced green hydrogen projects today are likely to use desalination [21]. Desalination is often seen as an expensive method for producing water, but in the context of hydrogen, it is a very small proportion of the costs (and energy consumption), only adding 0.02 to 0.05 USD/kg to the LCOH (i.e., circa 1% of LCOH today) [21]. Therefore, there is an opportunity to oversize desalination plants for green hydrogen projects. This concept has been announced for a green ammonia plant in Namibia, which has plans to oversize the desalination capacity in order to provide potable water to the nearby town of Luderitz [222]. For a country like India, safe drinking water is still a challenge. Nearly 200,000 Indians die each year because they lack access to safe drinking water, 60% of India's wastewater is released untreated, and 40% of the water supply is lost to leaks or theft [68]. The Indian government has prioritised getting a piped connection to drinking water to each house by 2024 via the Jal Jeevan Mission and established the Ministry of Jal Shakti to prioritise and coordinate water-related policies and activities [68]. The opportunity of additional desalination capacity needs to be further explored, but it is possible there could be significant benefits to oversizing capacity and providing water resilience to local communities.

In summary, it seems clear that based on scale that green hydrogen and ammonia will not cause a major new stress to the Indian water system. At the same time, there is an urgent imperative to improve water access and security in India. Coordinating the water infrastructure built for the hydrogen economy is crucial for preventing water stress and capturing water resilience opportunities.

6.3.3.3 Labour

The results of this thesis point towards potentially large shifts in labour markets from the energy transition. Today, the coal industry employs many people both formally and informally in India, with many of these labourers working in the poorest states in the Eastern Region [68]. For these people, coal extraction is the main economic activity available, and with a rapid decrease in the use of coal in this thesis's ESM as well as other rapid decarbonisation ESMs, there will be sudden unemployment of at least 500,000 formal workers and many more informal workers [68]. This type of transition, if not mitigated, can lead to social, economic, and political problems. On the other hand, there will be green sectors of the economy in which labour is increasing, such as grid expansion, clean power generation, EV manufacturing, efficiency improvements and retro-fitting, and new appliance manufacturing [68]. The government has prioritised domestic manufacturing of the key cost components of the energy transition, which is captured explicitly in the NHM for electrolysers and fuel cells. Industry is already announcing large domestic factories, such as Reliance Industry's 10 billion USD announcement in four giga-factories to produce batteries, solar PV modules, electrolysers, and fuel cells in Gujarat [223]. Opportunities for ensuring a smoother transition include prioritising the regions which are losing jobs as the sites of new manufacturing alongside other labour-intensive initiatives, e.g., environmental restoration projects in old mining regions [68].

The results of the grid connected scenarios of this thesis's ESM suggest that, despite the regional concentration of solar power generation in the Northern and Western regions, the production of hydrogen, ammonia, and the associated products do not need to be exclusively shifted to these regions. A simplified hydrogen and ammonia demand profile split equally across the regions found that transport infrastructure, via pipeline or shipping, should not be built to move hydrogen or ammonia, but rather transmission lines should be built to move electricity to produce hydrogen and ammonia in the local region of consumption. From a whole system level, this moving of electrons rather than molecules seems to be a lower cost solution, even if the LCOA was 10% to 20% more expensive in the Eastern Region compared to the Northern Region. Figure 6.5 highlights the regions where current hydrogen intensive industry is located, based on an analysis by TERI [2]. Refining and fertilisers are located on the coast, with proximity to imports of oil and LNG, as well as along the pipeline routes into the Northern centre of the country. The steel industry is concentrated near the coal mines in the Eastern Region. Further work is needed to understand the actual demand in each region, but these results point towards the potential for building out electrical transmission to connect regions, and building hydrogen and ammonia industry in all of the regions equally, and thus potentially easing the regional shifts of labour.

Finally, the results of the model suggest that ammonia production should ideally be very seasonal, which may cause challenges as labourers are generally looking for full time employment in high skilled chemical plants. There are examples of other similar industries which experience seasonal swings in production which should be researched for solutions, such as LNG regassification terminals in Europe. In the model, labour cost is included as a variable operating cost, and thus decreases with decreased ammonia production. This is likely a simplification, and if the labourers should instead be employed year round, their cost should be included as a fixed cost. Generally, however, operation and maintenance costs of green ammonia synthesis are relatively low, and thus this shift to fixed costs in the most conservative case would likely not change the results.

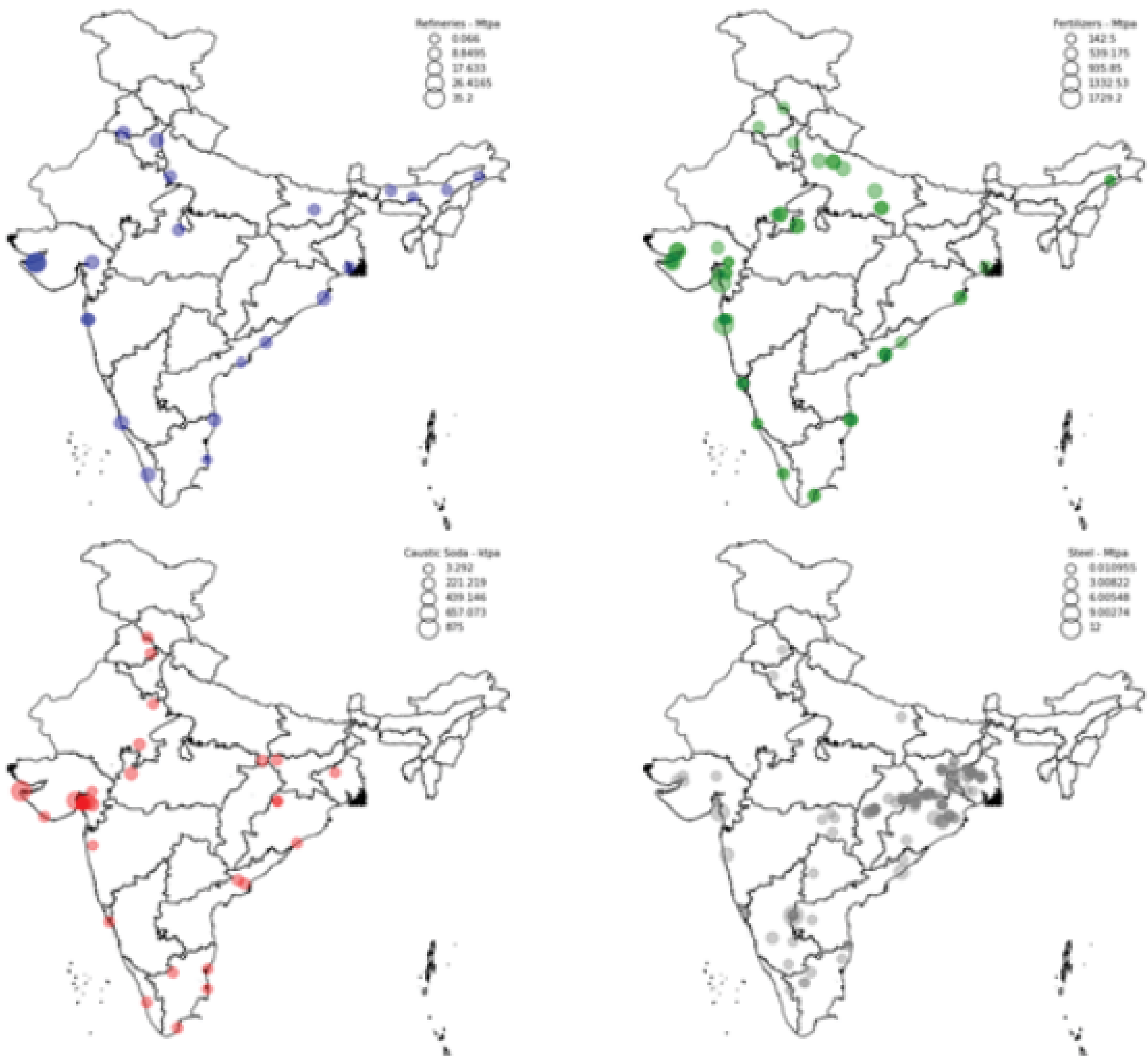


Figure 6.5: Geographical location of major industries susceptible to deployment of hydrogen, including refineries (upper left), fertilisers (upper right), caustic soda (lower left) and steel (lower right). From TERI [2].

6.4 Areas for improvement in the ESM methodology

There are several limitations of the sector coupled modelling which should be improved in future research. Five key limitations and improvements are highlighted for both the demand side and supply side modelling in this section.

6.4.1 Improving demand modelling

First, the demand for hydrogen and ammonia needs to be improved as better analysis and forecasts become available. Synthetic aviation fuel needs to be included in future models as it will likely have a similarly large sector coupling potential as shipping fuel. While it is unclear how much of the aviation demand can be met by biofuels or indeed which synthetic fuel(s) will be dominant, it would be better to include scenarios which include a flexible synthetic aviation fuel production process with storage, and update the model as the technological pathways become more evident. Additionally, the sectors included in the model may have higher demands for hydrogen and ammonia, as the demand scenario used in this analysis only considers 50% decarbonisation of steel and 60% of fertiliser production, as well as very low uptake of hydrogen FCEV in the heavy-duty vehicle sector. Therefore, the demand forecasts need to continuously be re-examined in future work. In the case of larger demands for green hydrogen and ammonia, such as for aviation fuel, the effect of storing fuels may be even more important in reducing the costs of the system.

Secondly, demand of the final products was taken to be flat across every hour of the year and equally distributed amongst the regions. This temporal simplification may be a misleading assumption for seasonally related sectors, such as fertilisers. Additionally, this assumption misses opportunity for seasonal trading in internationally connected sectors, e.g., marine bunker fuel or steel. India could export to the global commodity market in certain months, and import back from the market in other months to reduce the domestic storage requirements. Finally, the spatial simplification used in this ESM may create a false narrative about equal regional opportunity for production, and may cause different results regarding inter-regional fuel transport and transmission expansion if more detailed regional demand splits were used in the modelling.

Thirdly, to fully investigate the topic of chemical sector coupling, a deeper analysis of flexibility should be conducted, and the results incorporated into the model. No flexibility was assumed for steel production or other non-hydrogen industry demands (such as aluminium electrolysis), which may not be the case. This deeper dive into flexibility may also consider the costs and practicality of operating ammonia synthesis at minimum load for many months of the year. It is possible that there are alternatives to achieve the same results, such as building multiple smaller reactors which are seasonally turned off versus larger reactors which are seasonally turned down, but this analysis has not yet been done to date. Notably, ramping rates were not considered due to adding significantly to model calculation time, but since the value of chemical sector coupling is seasonal flexibility, this should not significantly affect the results.

Fourthly, along with better modelling of industrial flexibility, modelling of storage in non-electrical forms should be improved. The ESM currently only includes aboveground hydrogen storage and aboveground ammonia storage. Steel stockpiling or other forms of storage such as aluminium or synthetic aviation fuel were not included, but should be in future. Hydrogen cavern storage should also be included where appropriate.

Fifthly, the ESM excludes short duration sector coupling opportunities, such as in BEV and heating and cooling, which are well covered in other models and indeed in other iterations of Balmorel. This limitation causes an overestimate in the deployment in short duration batteries in the results. It is likely that the oversizing of batteries does not affect the long-duration storage results, which was the main focus of this ESM, but nevertheless the model should be expanded to include short duration sector coupling opportunities as well as long duration opportunities to fully capture the role of sector coupling.

6.4.2 Improving supply modelling

Similarly to demand, there are several supply side limitations which could be improved in future work.

First, the techno-economic evolution of new technologies must be monitored, and the ESM adapted to best capture imminent changes, such as underground hydrogen storage capabilities, cost estimates for ammonia gas turbines, small modular nuclear reactors, CDR technologies, CO_2 emission taxes, etc. A technology-rich ESM like Balmorel will always require frequent updates to the technology portfolio and cost assumptions to provide relevant research outputs.

Secondly, using ten years of historical weather data for the supply side data input is a step in the right direction, but likely insufficient. It is important for the system to be resilient to less frequent events as well as 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. Other forms of resilience, such as firm capacity, could also be modelled.

Thirdly, the economic and/or political cost of stranded assets is ignored in the model. The IEA forecasts that 83% of the coal and gas-fired plants in emerging economies will still have useful technical life in 2030, only reducing to 61% in 2040 [31]. As a result, countries are investigating co-firing of coal and gas plants with ammonia and hydrogen, or retrofitting them to run 100% on these green fuels. In the latest IEA Net-Zero scenario, the use of ammonia for co-firing in coal power stations globally in 2050 is 60 MMTPA and 140 TWh of electricity generation [31]. In a specific analysis of India, the IEA has investigated co-firing existing natural gas plants in the Eastern Region with 30% and 60% green hydrogen produced in the Southern Region and transported using existing natural gas pipeline infrastructure in India, which adds very little (c. 0.30 USD/kg) to the price of hydrogen [31]. These types of multi-fuel opportunities are not included in the ESM, although other Balmorel research has built add-ons to perform multi-fuel capabilities. Additionally, the costs of stranded assets are not adequately captured in the ESM to date, and more research is needed to consider how to best include this.

Fourthly, CDR is not considered as a technological option in the model. CDR technologies, like DAC with CCS and BECCS, create net negative emissions flows. In the context of this ESM, these flows can be useful in offsetting the emissions from dispatchable electricity, such as unabated natural gas peakers, which are infrequently used, as found in Bistline & Blanford [216]. Including this technology may affect the key results of the ESM by reducing ammonia-to-power with preference for natural gas and reducing the seasonality of ammonia production. However, since India's LNG import price is forecasted to be quite high, this technology may be less relevant for the Indian context, but more relevant for other countries.

Fifthly, as mentioned in the demand side potential for trading seasonally, there exists an opportunity to import chemicals and fuels, such as green ammonia, which was not included on the supply side. This limitation may be acceptable for the analysis of a country like India, where VRE is low cost on a global relative basis, but less acceptable for modelling other country contexts.

6.4.3 Other countries

In addition to addressing the limitations highlighted above, the sector coupled role of 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. The role of ammonia for seasonal balancing may be more significant in countries which are more wind dominated, such as the UK, because wind seasonality and interannual variations is often larger than solar (as found in modelling 39 years of weather data on India, see Figure 4.10). In the Indian context, wind was only 10% of the Indian electricity generation by 2050, and thus other more wind dominated case studies should be explored.

The results for the Indian system are demonstrative of certain trends, but ultimately, each regional ESM needs to include green hydrogen and ammonia sector coupling. Importantly, the ESM system in future work should be done at a large enough scale to capture the intertwined effects of industrial load shifting, transmission, and varying VRE resource availability. If the ESM is too geographically small, modelling will miss opportunities for optimal temporal shifting of inter-regional VRE resources. Models at a city or provincial level are unlikely to be useful for understanding electricity system planning. This challenge is easier to overcome in islanded contexts (such as Australia) or nations that are unlikely to trade significantly with neighbours, such as India and China, and harder to overcome in contexts like the EU with many individual actors as well as significant opportunities for trade.

6.5 Discussion on the model

Overall, the Balmorel model with OptiFlow add-on is an appropriate and useful model for answering this research's question. As highlighted in this Discussion chapter, there are many aspects of electricity system development that are not least-cost driven but instead depend on social, political and other considerations, and Balmorel is not a model intended to try to consider these real-world factors. Nevertheless, the more techno-economically steps of including sector coupling in an ESM and modelling different scenarios is well addressed in Balmorel.

The demand side limitations highlighted in this Discussion are: i) including new hydrogen, ammonia, or synthetic fuel demands, ii) assuming a non-flat demand for ammonia products over the year, iii) including the flexiblity from other insutries, like steel, iv) modelling of storage in non-electrical forms, and v) short duration sector coupling. Balmorel/OptiFlow can easily address i), iii), iv), and v) and indeed other instances of Balmorel focus on v). For ii), a challenge for this research was modelling the production minimum on the HB synthesis in OptiFlow. Ultimately, the simplification of flat demand over the weeks of the year was required based on the model structure. To remove this simplification, which is likely something that is worth removing in future research, it might be required to use a different model or updated version of OptiFlow.

The supply side limitations highlighted in this Discussion are: i) including new technology developments, ii) modelling more than 10 years of data and/or other forms of resilience, iii) including the economic and social cost of stranded assets, iv) including CDR technologies, and v) importing green fuels. Balmorel/OptiFlow can easily address i) and ii). For iii), the cost of decommissioning plants is not currently well represented in Balmorel, but further work could easily add this to the model. The social costs are not well represented, and could only be represented with some economic proxy value. For iv), CDR technologies should be possible to include, although significant model development of use of another vector in the OptiFlow add-on may be required. Finally, for v) Balmorel/OptiFlow should be able to easily consider availability of ammonia from the import market at certain times of the year, but the actual modelling of this availability would need to be done externally and used as an exogenous availability in Balmorel/Optiflow.

There are several other challenges in using Balmorel that were encountered in the course of this research that may be worth highlighting for future work.

One challenge is that Balmorel is only set up to model 8,760 hours per year. This was challenging for modelling many years of weather data and answering research sub-question 3. A functional work-around was discovered for modelling 10 years of weather data in the operation simulation part of the model, using a total of 3,536 timesteps per 1 year of operation simulation. This will continue to work for modelling approximately 25 years of data at the same granularity as this research, but fewer years if a researcher wants to increase the temporal granularity. At some point the number of timesteps may exceed 8,760 and this will likely require changes to deeper layers of the code. This is almost certainly possible, as one has access to all of the files very easily in Balmorel, but potentially requiring significant debugging time as the files are long and full of many variables.

A second challenge with using Balmorel was that the run time was long. This was a major challenge in this research for debugging, iterating, and running sensitivities. Possibly future work with Balmorel should consider investigating computational options, ranging from procuring improved computing power to relaxing some optimisation thresholds. It is possible that other models are set up in a more efficient manner, but it is outside of the scope of this research to speculate on this.

A third challenge, which is likely not unique to Balmorel, is working on a model of a country by oneself, without other active users. It would have been helpful to have other modellers actively modelling India in Balmorel to help catch small bugs along the way. This is a potential reason to shift to Open Source models that are also using free software and rapidly attracting users, like PyPSA.

7 | Conclusions

This thesis aims to better understand the future role of green ammonia, a rapidly emerging technology, in the broader energy system and specifically the electricity system. The findings call the energy system research community's attention to the transformational effects of hydrogen and ammonia sector coupling in a future grid design, and shine a light on lower cost, more resilient system designs. This analysis works towards filling the gap in the literature on dynamic, deep hydrogen and ammonia sector coupling. India is used as a case study, but the methodology and findings are generally applicable. Furthermore, India is an important case study for a global audience due to its prominence on the global scale. This thesis is targeted towards the policymakers who are deciding *today* about hydrogen roadmaps, as well as the energy system modellers around the world who are informing these policymakers and businesses about deep decarbonisation pathways. This conclusion chapter restates the research questions introduced in Chapter 1 and provides a succinct answer based on the findings. The novel contributions are summarised, key limitations highlighted, and future research pathways set forth.

7.1 Restatement of Research Objectives with Summarised Key Findings

The main research question of this thesis was, "**Which significant roles will green ammonia have in decarbonised electricity systems?**" Ultimately, this thesis concludes that ammonia's key roles in a decarbonised energy system, from most certain to least certain, are:

1. Sector coupling of flexible green ammonia production and bulk storage for electricity system seasonal load-shifting

2. Sector coupling of flexible green ammonia production and bulk storage for provision of electricity system resilience to interannual VRE variation

3. Dispatchable power generation via ammonia-to-power for seasonal variation and inter-annual variation at high VRE penetrations

Three sub-questions are answered to develop a more complete answer to this research question.

Sub-question 1: Should green ammonia be used for re-electrification in power grids? How does using green ammonia for dispatchable power generation compare with traditionally modelled low-carbon technologies for dispatchable power, such as fossil fuel with Carbon Capture and Storage (CCS), nuclear energy, and bioenergy with or without CCS?

Standalone models of power-to-ammonia and ammonia-to-power were developed to provide a LCOA and LCOE foundation for comparing power-to-ammonia-to-power to traditional technologies. Then, a capacity expansion and dispatch ESM of the Indian system was developed to understand the role of power-to-ammonia-to-power compared to other technologies in the electricity system to 2050. The results of the LCOA and LCOE analyses suggest that ammonia is a viable alternative fuel for power generation by 2040, with ammonia LCOA declining steadily to levels in the range of natural gas prices. Ammonia cracking, if required for gas turbine power generation, is found to add modest additional costs to the LCOE. Ammonia-to-power is found to be markedly more favourable than traditionally modelled low-carbon technologies, like post-combustion CCS, nuclear, and BECCS, at power plant utilisation less than 25%. Utilisation under 25% is expected for the roles of seasonal balancing, peaking, and resilience in the power system. In the ESM of the Indian power system, power-to-ammonia-to-power is used in most scenarios, but it contributes less than 1% of the power to the grid by 2050. While the role in India for power-to-ammonia-to-power seems relatively small, the results are consistent with the hypotheses of using ammonia for seasonal storage and resilience, and therefore suggest that ammonia-to-power should be investigated in ESM of other countries and contexts.

Sub-question 2: What are the effects of "sector coupling" green ammonia production (for various non-power sector users such as maritime shipping fuel and fertiliser) with the electricity grid system? Should green ammonia production be grid connected or islanded?

The aggregated green hydrogen and ammonia demand across sectors in the Indian context is found to amount to 25% of the electricity demand by 2050. This level is consistent with IRENA's estimate of 30% of global electricity demand being used to make hydrogen and its derivates by 2050 in a 1.5 C compatible scenario [21].

The striking conclusion of the ESM analysis of India is that green ammonia, with its low cost of above-ground storage and potential for process flexibility, can and should be used to provide seasonal demand side load-shifting. This demand load-shifting and seasonal stockpiling of ammonia significantly reduces the cost of the entire energy system, reduces LCOH and LCOA, reduces curtailment, reduces the demand for long-duration storage and dispatchable electricity, and improves system resilience. In the sector-coupled scenarios' results, ammonia production mostly occurs from March until August, with production reduced to minimum technical levels outside of these months. 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 is then stored in large quantities (15 to 40 MMT) in aboveground stockpiles for meeting the annual demand. This type of seasonal storage is similar to current practices of storing natural gas for winter use in European countries. Additionally, smaller amounts of hydrogen storage are found to be useful for short-duration load shifting in the sector coupled scenarios.

Hydrogen and ammonia transport are not found to be deployed in any scenario. The results instead show investment to increase transmission capacity to move electricity across distances and then locally produce hydrogen and ammonia for regional consumption.

Ammonia-to-power is also used at small levels in most scenarios for seasonal peaking and resilience to unfavourable interannual VRE variation. Factors which would cause more ammonia to be used include higher penetrations of wind generation compared to solar, more weather years of input data capturing more interannual variation, decoupled sectors especially for seasonal load-shifting of demand, and stricter restrictions on CO_2 emissions. Interestingly, over-building solar PV with battery, in all but the most favourable cost scenarios for solar PV and batteries, is found to be less cost optimal than having some reserve of ammonia-to-power to provide system resilience.

In summary, in the Indian context, ammonia-to-power plays a minor role, while the more prominent effect of sector coupling of hydrogen and ammonia is the seasonal load-shifting of production and large above-ground storage of ammonia.

Sub-question 3: What are the effects of grid resilience on both potential roles (power-to-ammonia and ammonia-to-power), as explored via seasonal and interannual variation of solar PV and wind energy?

In the results of the Indian ESM, most of the seasonal variation is absorbed via flexible ammonia production, and only the scenarios without access to grid connected ammonia production use ammonia-to-power for annual seasonal balancing. The seasonality in the Indian grid is largest in the wind power profiles; however, only 10% of power generation in the system is wind in 2050 with the remainder being solar, which experiences less seasonality. Therefore, the role of ammonia-to-power in balancing seasonal variation may be more pronounced in future research on other countries which are more wind dominated, such as the UK.

Interannual variation, on the other hand, does cause ammonia-to-power to be deployed in almost all scenarios as the least-cost form of resilience to unfavourable weather years. Ten years of historical weather data were used in the Indian ESM, and significant differences between the years can be observed, notably in the use of ammonia-to-power and the level of stockpiled ammonia in the reserve.

7.2 Contribution

Hydrogen and ammonia are on the cusp of mass deployment into energy systems around the world. This thesis shines a light on the role of ammonia specifically, which is researched far less than hydrogen. First, this research filled gaps in foundational models of power-to-ammonia and ammonia-to-power. Secondly, this research developed the first ESM to include hydrogen and ammonia demands in industrial and synthetic fuel sectors at the scale they are likely to assume (c. 25% of electricity demand) and with flexible production and storage so that seasonal load shifting is possible. Since no other ESM in the literature have captured these elements, the literature to date is missing this significant opportunity to reduce costs, reduce long-duration storage, and improve resilience via hydrogen and ammonia load-shifting. Additionally, this is the first ESM to quantify the extent to which hydrogen and ammonia will be needed for dispatchable electricity generation in India.

7.3 Limitations and Future Research

Improvements to the ESM are detailed in Chapter 5, but several of the thesis's most important limitations and areas of future research are summarised here.

First, the general trends and roles of ammonia are explored in the case study on India, but applying the results to other countries is not straightforward: a country or regional level ESM analysis is required to understand the interplay of electricity demand, hydrogen and ammonia demand, VRE supply mix, transmission, interannual variation, etc. Future work should apply this ESM to other geographies to validate the results of the Indian case study and observe any effects which are not found in the Indian case study. Since it takes significant effort to build high quality ESMs, there may be opportunities to collaborate. Project partners on the EEIST project in China use Balmorel for modelling China to 2050, which may be a good second case study. Additionally, collaborators from DTU use Balmorel to study European energy systems, which are somewhat more difficult to model due to many national actors, but nevertheless important and a good next case study for this research.

Secondly, resilience was modelled using ten years of historical weather data; however, 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 (i.e., ammonia-to-power) and should be considered in future work as climate models are able to provide this data. Also, alternative methods of modelling resilience beyond multiple weather years should be explored, such as firm reserve capacity.

Thirdly, this analysis does not consider trade of green ammonia with other countries, which is likely to be significant by 2050. For the case study of India, international trade may be less relevant as India is well positioned to export green ammonia at very competitive prices. However, this would not be true of other countries, such as European countries, and therefore would need to be included.

Fourthly, there are several simplifications and limitations in the data for India which, although acceptable for drawing out the key results of this thesis, could be further improved, especially with a modelling partner in India. For example, India itself may have higher demands for hydrogen and ammonia, as the demand scenario used in this analysis only considers 50% decarbonisation of steel and 60% of fertiliser production, and does not consider synthetic fuels for aviation. Additionally, a deeper, cross-disciplinary analysis of chemical sector flexibility should be conducted on both the included sectors of fertiliser and shipping fuel, as well as other sectors not included, such as green steel production and aluminium electrolysis. This work points towards stockpiling ammonia for fertiliser and shipping fuel as unconventional forms of seasonal energy storage, and there is no reason other forms, e.g., piles of steel and aluminium, should not also be considered.

Finally, there exist fundamental uncertainties and complexities that limit one's ability to predict the exact mix of future energy systems. The real value of models such as the one presented here is not the precise results of an ESM looking toward 2050, but rather to highlight leverage or sensitive intervention points [224] and system designs which dramatically alter the end-state of the system transformation. This thesis finds that hydrogen and ammonia sector coupling *can* be one point of leverage to change electricity grids for the better. It is the author's hope the analysis presented here motivates and accelerates the wider research community into expanding ESMs to consider the potential impacts of hydrogen and ammonia in decarbonised energy systems.

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A | Appendix

A.1 Data input tables for models

Table A.1: GSAM techno-economic input assumptions

	Year						
Component technical/economic assumption	2020	2025	2030	2035	2040	Unit note: 2019USD	Reference
Solar PV (single axis tracking)							
Solar installed CAPEX	576	493	410	386	363	USD/ MWp_{DC}	DEA [87]
Global Horizontal Irradiance (GHI)	2,000	2,000	2,000	2,000	2,000	kWh/m2/yr	Global Solar Atlas[139]
Performance ratio (measure of combined losses)	0.86	0.91	0.95	0.96	0.96		DEA[87]
Capacity Factor (fixed tilt, DC rating)	0.2	0.21	0.22	0.22	0.22	%	Calculated
DC/AC Sizing Factor (also called Inverter Loading Ratio)	1.25	1.25	1.25	1.25	1.25	W_{DC}/W_{AC}	DEA[87] and high insolation regions (greater than1,890 GHI) with single axis tracking average 1.28 [141]
Capacity Factor (fixed tilt, AC rating)	0.25	0.26	0.27	0.27	0.27	%	Calculated. Agrees with high insolation regions in USA [141]
Single axis tracking increase to capacity factor	0.05	0.05	0.05	0.05	0.05	%	High insolation regions show up to 5% point increase to capacity factor due to single axis tracking [141]
Capacity Factor (single axis tracking, AC rating)	30%	31%	32%	32%	32%	%	Calculated, and agrees with 2018 average of 30.4% with range up to 34% in high insolation regions in USA [141]
Solar single axis tracking average annual full load hours (AC rating)	2,588	2,701	2,813	2,826	2,838	kWh/yr/kW_{AC}	Calculated
O&M	7,400	6,800	6,200	5,950	5,700	USD/ MWp_{DC} /yr	DEA[87]
LCOE	28.5	23.6	19.1	18	16.8	USD / MWh	Calculated
Electrolyser							
Electrolyser CAPEX	770	655	540	488	435	USD / kW input	IRENA 2020 Global Renewables Outlook[143]
Efficiency [LHV of H_2]	64%	67%	69%	72%	74%	%	IEA[24]
O&M	1.5%	1.5%	1.5%	1.5%	1.5%	% of CAPEX	IEA[24]
Stack Lifetime (operating hours)	95,000	95,000	95,000	100,000	100,000	hr	IEA[24]
Ammonia Synthesis							
Haber-Bosch CAPEX	3,300	3,300	3,300	3,300	3,300	USD/kg NH_3/hr	[80]
Air Separation Unit (ASU) CAPEX	1,450	1,450	1,450	1,450	1,450	USD/kg N_2/hr	[80]
Haber-Bosch electricity consumption	0.6	0.6	0.6	0.6	0.6	MWh/t NH_3	[71]
ASU electricity consumption	0.119	0.119	0.119	0.119	0.119	MWh/t N_2	[71]
H_2 Storage required for HB Management	2	2	1.5	1	1	days at full load	Modified from [76]
Hydrogen Storage							
Aboveground (200 bar w/o compressors) CAPEX	1,050	961	872	743	615	USD/kg	DEA [144]
Lithium Ion Battery							
CAPEX (Energy Component)	271	218	166	138	110	USD / kWh	DEA [144]
CAPEX (Power Component)	315	251	187	152	117	USD / kW	DEA [144]
Fixed O&M	631	631	631	631	631	USD/ MW/yr	DEA [144]
Variable O&M	2.3	2.2	2.1	2	2	USD / MWh	DEA [144]
Desalination							
Installed CAPEX	5.72	5.72	5.72	5.72	5.72	USD/m^3/yr	[225] assuming mechanical vapor compression from [51]
Financing							
Weighted Average Cost of Capital (WACC)	7.5%	7.5%	7.5%	7.5%	7.5%	%	[146]
Economic lifetime	25	25	25	25	25	years	

Table A.2: LCOE techno-economic assumptions

		Unit	Reference
General assumptions			
Plant size	1,000	MW	UK BEIS & Uniper [205]
Power plant capacity factor	25%	%	Identified as approximate capacity factor for technology required for 2°C decarbonization in [24]
WACC	7.5%	%	Standard used in IRENA for OECD and China [146]
CO_2 Price	140	USD/t CO_2	IEA advanced economies power sector forecasted CO_2 price in 2040 [145]
Fuel Price in 2040			
Natural Gas	8.9	USD/ MMBTU	EU price forecast 2040 in IEA STEPS scenario [145]
Coal	78	USD/t	EU price forecast 2040 in IEA STEPS scenario [145]
Green Ammonia	380	USD/t NH3	Fig. 5a
Biomass	8.0	USD/GJ	ESME for Biomass imports mid-range 2050 [90]
Coal + CCS			
Supercritical plant fuel efficiency (LHV)	41%	%	Global CCS Institute[226]
CAPEX	2,328	USD / kW	Global CCS Institute[226]. No future progress assumed on Rankine cycle CAPEX or efficiency, in line with IEA[145]
Economic Lifetime	30	years	[90]
Plant fuel efficiency with CCS (LHV)	33%	%	Global CCS Institute[226]
CCS additional CAPEX	1,426	USD / kW	Global CCS Institute [226]
Fixed O&M with CCS	64,912	USD/ MW/yr	Global CCS Institute[226]
Variable O&M with CCS	19	USD / MWh	Global CCS Institute[226]
Lifecycle emissions before CCS	797	kg CO_2/ MWh	Average of Global CCS Institute[226] (774 kg CO_2/ MWh) and IPCC [227] (820 kg CO_2/ MWh)
Lifecycle emissions after CCS	159	kg CO_2/ MWh	Average of Global CCS Institute[226] (97 kg CO_2/ MWh) and IPCC [227](220 kg CO_2/ MWh)
Gas CCGT + CCS			
CCGT plant fuel efficiency (LHV)	60%	%	UK BEIS & Uniper [205]. No future progress assumed on GT CAPEX or efficiency, in line with IEA[145]
CAPEX	766	USD / kW	UK BEIS & Uniper [205]. No future progress assumed on GT CAPEX or efficiency, in line with IEA[145]. Also matches developing country costs [83]
Lifetime	25	years	UK BEIS & Uniper [205]
Plant fuel efficiency with CCS (LHV)	53%	%	UK BEIS & Uniper [205]
CCS additional CAPEX	1116	USD / kW	UK BEIS & Uniper [205]
Fixed O&M with CCS	42,225	USD/ MW/yr	UK BEIS & Uniper [205]
Variable O&M with CCS	11	USD / MWh	UK BEIS & Uniper [205]
Lifecycle emissions before CCS	490	kg CO_2/ MWh	IPCC [227]including methane emissions CO_2 equivalent
Lifecycle missions after CCS	170	kg CO_2/ MWh	IPCC [227]including methane emissions CO_2 equivalent.
CCS CAPEX reductions in future	30%	%	UK BEIS & Uniper [205]
Lifecycle emissions after CCS in future	94	kg CO_2/ MWh	IPCC [227]minimum range of estimates for present day technology, including methane emissions CO_2 equivalent.
Ammonia CCGT			
CCGT plant fuel efficiency (LHV)	60%	%	Assuming same as NG [205]
CAPEX	766	USD / kW	Assuming same as NG [205]
Lifetime	25	years	Assuming same as NG [205]
Fixed O&M	17,353	USD/ MW/yr	Assuming same as NG [205]
Variable O&M	5	USD / MWh	Assuming same as NG [205]
Ammonia CCGT with Cracker			
Cracker conversion	99%	% of NH3	99% conversion at 850 °C based on small-scale commercial crackers using nickel catalysts [54], [55].
Cracker output recycle size	20.5%	% of output	Calculated using ASPEN Plus
H2 separation losses	1%	%	Based on 80–85% recovery via H2 membrane [79] and tail gas used for recycle, so very small losses
Phase 1			
Cracker size	63.7	ton H2/hr	Calculated using ASPEN Plus
Plant fuel efficiency with cracker (LHV)	53.8%	%	Calculated using ASPEN Plus
Cracker additional CAPEX	402	USD / kW	Calculated using Cracker cost curve from Figure 3.9
Phase 2			
Cracker size	17.3	ton H2/hr	Calculated using ASPEN Plus
Plant fuel efficiency with cracker (LHV)	58.0%	%	Calculated using ASPEN Plus
Cracker additional CAPEX	152	USD / kW	Calculated using Cracker cost curve from Figure 3.9
Nuclear			
Fuel Cost	4	USD / MWh	World Nuclear Association [89]
CAPEX	4,500	USD / kW	EU CAPEX in IEA's 2040 forecast[145]
Economic Lifetime	30	years	[90]
Fixed O&M	100,000	USD/ MW/yr	EIA [88]

Continuation of Table A.2			
		Unit	Reference
Bioenergy with CCS			
BECCS plant fuel efficiency (LHV)	37%	%	ESME- biomass-dedicated steam turbine power station [90]
CAPEX	3,653	USD / kW	ESME [90]
Lifetime	30	years	ESME [90]
Fixed O&M with CCS	140,492	USD/ MW/yr	ESME [90]
Variable O&M with CCS	7	USD / MWh	ESME [90]
Negative CO_2 emissions	0.35	$GtCO_2/EJ$	Mean value from Fuss et al range of 0.02–0.05 $GtCO_2/EJ$ [73]
Negative CO_2 emissions (electricity)	342	kg CO_2 / MWh	Calculated based on 37% efficiency

Table A.3: Monthly electricity demand by region in 2020

	NR	SR	WR	ER	NER	Unit
Jan	56.0	52.3	60.9	16.3	2.8	TWh/yr
Feb	48.9	50.4	53.7	15.9	2.5	TWh/yr
Mar	54.1	59.7	62.2	19.9	2.6	TWh/yr
Apr	54.8	52.0	61.3	19.4	2.4	TWh/yr
May	66.3	50.4	61.4	19.2	2.6	TWh/yr
Jun	66.4	44.3	54.2	18.7	2.9	TWh/yr
Jul	70.5	48.3	50.7	18.6	3.0	TWh/yr
Aug	71.2	48.3	54.8	19.3	3.3	TWh/yr
Sep	66.7	46.3	55.2	19.6	3.0	TWh/yr
Oct	61.3	45.7	60.4	18.7	3.0	TWh/yr
Nov	50.1	47.5	60.5	15.1	2.6	TWh/yr
Dec	52.9	50.1	61.0	15.1	2.7	TWh/yr

A.2 ESM results tables

Table A.4: Indian LCOH and LCOA by scenario to 2050

	2030	2040	2050	Unit
LCOH				
Connected - Historical Mix	1.75	1.53	1.72	USD/kg H_2
Connected - Slow Transition	1.51	0.98	0.87	USD/kg H_2
Connected - Fast Transition	1.14	0.65	0.65	USD/kg H_2
Islanded - Historical Mix	2.86	2.37	2.12	USD/kg H_2
Islanded - Slow Transition	2.46	1.49	1.11	USD/kg H_2
Islanded - Fast Transition	1.86	0.99	0.79	USD/kg H_2
LCOA				
Connected - Historical Mix	499	430	443	USD/t NH_3
Connected - Slow Transition	461	298	262	USD/t NH_3
Connected - Fast Transition	365	219	211	USD/t NH_3
Islanded - Historical Mix	629	545	497	USD/t NH_3
Islanded - Slow Transition	545	368	296	USD/t NH_3
Islanded - Fast Transition	433	269	233	USD/t NH_3

Table A.5: Curtailment results across years and scenarios (TWh/yr)

Year	Scenario	Hydro Reservoir	Hydro River	Small Hydro	Solar	Offshore Wind	Onshore Wind	Total Curtailment	Total Generation	% curtailment
2020	Connected, Hist.	48	1	0	-	-	-	48	1,161 4.2%	
	Connected, Slow	48	1	0	-	-	-	48	1,161 4.2%	
	Connected, Fast	48	1	0	-	-	-	48	1,161 4.2%	
	Islanded, Hist.	48	1	0	-	-	-	48	1,161 4.2%	
	Islanded, Slow	48	1	0	-	-	-	48	1,161 4.2%	
	Islanded, Fast	48	1	0	-	-	-	48	1,161 4.2%	
2030	Connected, Hist.	91	0	0	0	1	191	283	2,213 12.8%	
	Connected, Slow	92	4	1	4	1	116	217	2,251 9.6%	
	Connected, Fast	93	9	2	30	1	85	221	2,282 9.7%	
	Islanded, Hist.	91	1	0	4	1	226	323	2,211 14.6%	
	Islanded, Slow	93	8	2	12	1	146	262	2,249 11.7%	
	Islanded, Fast	91	14	3	42	1	103	254	2,281 11.1%	
2040	Connected, Hist.	93	14	4	109	1	189	409	4,447 9.2%	
	Connected, Slow	94	15	4	162	1	206	482	4,437 10.9%	
	Connected, Fast	95	19	4	230	1	236	584	4,434 13.2%	
	Islanded, Hist.	94	19	5	172	1	261	553	4,447 12.4%	
	Islanded, Slow	96	23	6	268	2	259	653	4,443 14.7%	
	Islanded, Fast	93	27	5	380	2	293	800	4,441 18.0%	
2050	Connected, Hist.	94	19	5	423	1	185	727	7,405 9.8%	
	Connected, Slow	95	19	5	534	1	212	866	7,379 11.7%	
	Connected, Fast	95	21	4	630	1	243	994	7,361 13.5%	
	Islanded, Hist.	96	28	7	635	2	313	1,081	7,429 14.5%	
	Islanded, Slow	97	28	7	850	2	312	1,295	7,377 17.6%	
	Islanded, Fast	94	29	6	959	2	367	1,457	7,360 19.8%	

Table A.6: Annual system costs on 2050 across scenarios (USD Bn)

	Solar PV	Battery	Wind	H_2 Syn	NH_3 Syn	NH_3 GT	Hydro	Nuclear	Biomass	Transmission	Total	El Price (USD/MWh)
Connected, Hist.	169	79	43	31	16	5	7	6	1	1	358	47.3
Connected, Slow	122	40	32	14	12	1	6	4	1	1	232	27.5
Connected, Fast	92	33	28	10	11	-	5	3	1	1	184	22.2
Islanded, Hist.	176	84	49	31	13	7	7	12	2	0	381	49.2
Islanded, Slow	130	45	32	14	11	4	6	3	1	0	245	28.3
Islanded, Fast	98	37	28	10	10	2	5	3	1	0	193	22.9

Table A.7: Generation from dispatchable resources from 2020 to 2050 across scenarios (TWh)

	Scenario	Biomass	Coal	Hydro Reservoir	Natural Gas	Nuclear	NH_3	Total Dispatchable	Total curtail.	Total Gen	Total Gen w/o curtail.	% dispatchable	% NH_3
2020	Connected, Hist.	0	841	138	0	0	0	979	48	1,161	1,112	88%	0.0%
	Connected, Slow	0	841	138	0	0	0	979	48	1,161	1,112	88%	0.0%
	Connected, Fast	0	841	138	0	0	0	979	48	1,161	1,112	88%	0.0%
	Islanded, Hist.	0	841	138	0	0	0	979	48	1,161	1,112	88%	0.0%
	Islanded, Slow	0	841	138	0	0	0	979	48	1,161	1,112	88%	0.0%
	Islanded, Fast	0	841	138	0	0	0	979	48	1,161	1,112	88%	0.0%
2030	Connected, Hist.	47	89	248	83	79	0	547	283	2,213	1,930	28%	0.0%
	Connected, Slow	40	32	237	79	80	0	468	217	2,251	2,034	23%	0.0%
	Connected, Fast	31	9	223	48	74	0	386	221	2,282	2,061	19%	0.0%
	Islanded, Hist.	47	112	245	78	72	0	555	323	2,211	1,888	29%	0.0%
	Islanded, Slow	44	36	226	78	71	0	455	262	2,249	1,987	23%	0.0%
	Islanded, Fast	35	11	203	56	67	0	373	254	2,281	2,027	18%	0.0%
2040	Connected, Hist.	22	0	224	30	128	14	417	409	4,447	4,038	10%	0.4%
	Connected, Slow	8	0	216	8	58	2	293	482	4,437	3,954	7%	0.1%
	Connected, Fast	4	0	210	5	46	0	265	584	4,434	3,850	7%	0.0%
	Islanded, Hist.	22	0	212	37	129	19	420	553	4,447	3,894	11%	0.5%
	Islanded, Slow	14	0	200	15	56	5	289	653	4,443	3,789	8%	0.1%
	Islanded, Fast	6	0	180	6	38	2	232	800	4,441	3,641	6%	0.0%
2050	Connected, Hist.	10	0	217	0	109	11	347	727	7,405	6,677	5.2%	0.2%
	Connected, Slow	2	0	208	0	42	2	255	866	7,379	6,513	3.9%	0.0%
	Connected, Fast	1	0	205	0	36	0	243	994	7,361	6,367	3.8%	0.0%
	Islanded, Hist.	14	0	199	0	98	29	340	1081	7,429	6,348	5.4%	0.5%
	Islanded, Slow	5	0	188	0	25	8	227	1295	7,377	6,081	3.7%	0.1%
	Islanded, Fast	3	0	172	0	16	4	195	1457	7,360	5,902	3.3%	0.1%

Table A.8: Installed capacity from 2020 - 2050 across scenarios (GW)

		Coal	Natural Gas	Nuclear	Hydro	Solar	Wind	Biomass	NH_3	Battery	Pumped Hydro	Total
2020	Connected, Hist.	197	24	9	47	22	34	8			4	345
	Connected, Slow	197	24	9	47	22	34	8			4	345
	Connected, Fast	197	24	9	47	22	34	8			4	345
	Islanded, Hist.	197	24	9	47	22	34	8			4	345
	Islanded, Slow	197	24	9	47	22	34	8			4	345
	Islanded, Fast	197	24	9	47	22	34	8			4	345
2030	Connected, Hist.	202	24	13	81	388	375	10		58	5	1157
	Connected, Slow	202	24	13	74	618	254	10		173	5	1374
	Connected, Fast	202	24	13	72	842	163	10		260	5	1592
	Islanded, Hist.	202	24	13	81	411	372	10		63	5	1182
	Islanded, Slow	202	24	13	73	659	251	10		183	5	1422
	Islanded, Fast	202	24	13	69	872	163	10		269	5	1629
2040	Connected, Hist.		24	22	82	1827	399	10	44	524	5	2938
	Connected, Slow		24	22	74	2055	334	10	13	642	5	3180
	Connected, Fast		24	22	72	2143	334	10		674	5	3286
	Islanded, Hist.		24	38	82	1901	409	10	50	526	5	3046
	Islanded, Slow		24	22	74	2167	334	10	22	691	5	3350
	Islanded, Fast		24	22	69	2288	334	10	6	728	5	3488
2050	Connected, Hist.			22	82	3829	399	10	49	946	5	5341
	Connected, Slow			22	74	4074	334	10	13	1043	5	5575
	Connected, Fast			22	72	4151	334	10		1056	5	5651
	Islanded, Hist.			38	82	3973	458	10	69	1014	5	5650
	Islanded, Slow			22	74	4343	334	10	34	1197	5	6020
	Islanded, Fast			22	69	4446	334	10	21	1222	5	6130

Table A.9: Annual power generation from 2020 - 2050 across scenarios (TWh/yr)

		Coal	Natural Gas	Nuclear	Hydro	Solar	Wind	Biomass	NH_3	Battery	Pumped Hydro	Total w/o Storage	Wind %	Solar %
2020	Connected, Hist.	841	0	0	230	35	55	0	0	0	0	1161	5%	3%
	Connected, Slow	841	0	0	230	35	55	0	0	0	0	1161	5%	3%
	Connected, Fast	841	0	0	230	35	55	0	0	0	0	1161	5%	3%
	Islanded, Hist.	841	0	0	230	35	55	0	0	0	0	1161	5%	3%
	Islanded, Slow	841	0	0	230	35	55	0	0	0	0	1161	5%	3%
	Islanded, Fast	841	0	0	230	35	55	0	0	0	0	1161	5%	3%
2030	Connected, Hist.	89	83	79	399	691	825	47	0	131	7	2213	37%	31%
	Connected, Slow	32	79	80	357	1078	585	40	0	376	6	2251	26%	48%
	Connected, Fast	9	48	74	330	1427	363	31	0	575	6	2282	16%	63%
	Islanded, Hist.	112	78	72	395	726	780	47	0	125	7	2211	35%	33%
	Islanded, Slow	36	78	71	339	1136	544	44	0	370	6	2249	24%	51%
	Islanded, Fast	11	56	67	305	1464	342	35	0	571	6	2281	15%	64%
2040	Connected, Hist.	0	30	128	361	2997	895	22	14	1214	5	4447	20%	67%
	Connected, Slow	0	8	58	322	3319	719	8	2	1366	5	4437	16%	75%
	Connected, Fast	0	5	46	306	3392	682	4	0	1343	6	4434	15%	76%
	Islanded, Hist.	0	37	129	342	3055	842	22	19	1139	6	4447	19%	69%
	Islanded, Slow	0	15	56	297	3401	655	14	5	1382	7	4443	15%	77%
	Islanded, Fast	0	6	38	266	3492	632	6	2	1410	7	4441	14%	79%
2050	Connected, Hist.	0	0	109	348	6028	898	10	11	2263	5	7405	12%	81%
	Connected, Slow	0	0	42	309	6310	713	2	2	2382	6	7379	10%	86%
	Connected, Fast	0	0	36	298	6350	675	1	0	2376	6	7361	9%	86%
	Islanded, Hist.	0	0	98	318	6054	915	14	29	2231	6	7429	12%	81%
	Islanded, Slow	0	0	25	279	6457	602	5	8	2464	7	7377	8%	88%
	Islanded, Fast	0	0	16	255	6525	557	3	4	2506	8	7360	8%	89%

Table A.10: Transmission capacity from 2020-2050 across scenarios (GW)

	Connected, Hist.	Connected, Slow	Connected, Fast	Islanded, Hist.	Islanded, Slow	Islanded, Fast
2020	121	121	121	121	121	121
2030	129	121	121	121	121	121
2040	139	126	121	128	121	121
2050	210	198	194	145	137	132

A.3 Other Research contributions

Power-to-X literature review In addition to developing models, this research has also produced several higher level literature review and analysis publications. Specifically, a white-paper was published in collaboration with industry (Z. Cesaro, I. Wilkinson and A. Eisfelder, "Power-to-X: A Closer Look at E-ammonia," Siemens Energy, Technical Papers, 2020. [4]) to review green ammonia production and potential roles in decarbonised energy and chemical sectors.

Additionally, one book chapter was published to frame ammonia in the wider Power-to-X field (**Z. Cesaro**, R. M. Nayak-Luke and R. Bañares-Alcántara, "Chapter 2 - Energy Storage Technologies: Power-to-X," in Techno-Economic Challenges of Green Ammonia as an Energy Vector, Academic Press, 2020, pp. 15-26.), and another chapter was co-authored with contributions to the international perspectives of green ammonia uptake (R.M. Nayak-Luke, **Z. Cesaro**, R. Bañares-Alcántara, “Chapter 3 - Pathways for Green Ammonia,” in Techno-Economic Challenges of Green Ammonia as an Energy Vector, Academic Press, 2020, pp. 27-39.).

LCOE and LCOA modelling Further variations and parts of this research were published in the two book chapters: 1) R.M. Nayak-Luke, C. Forbes, **Z. Cesaro**, R. Bañares-Alcántara, K.H.R. Rouwenhorst, “Chapter 8 - Techno-Economic Aspects of Production, Storage and Distribution of Ammonia,” in Techno-Economic Challenges of Green Ammonia as an Energy Vector, Academic Press, 2020, pp. 191-207.; and 2) **Z. Cesaro**, J. Thatcher, R. Bañares-Alcántara, “Chapter 9 - Techno-Economic Aspects of the Use of Ammonia as Energy Vector,” in Techno-Economic Challenges of Green Ammonia as an Energy Vector, Academic Press, 2020, pp. 209-219.