Optimising Renewable Generation Configurations of Off-Grid Green Ammonia Production Systems considering Haber-Bosch Flexibility†

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Highlights

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- High-potential Australian hydrogen hubs with existing critical infrastructure are identified.
- A hybrid wind and solar PV generation system and/or partially flexible Haber-Bosch can reduce the need for storage considerably.
- A levelised cost of ammonia of AU$756/tonne and AU$659/tonne in 2025 and 2030, respectively, is calculated at the most favourable hubs.
- Green ammonia produced in Australia in 2030 would be cost-competitive with grey ammonia if the feedstock gas price is higher than AU$14/MBtu (without a carbon price).
- Potential synergy between southern hemisphere supply and northern hemisphere demand is highlighted.

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Abstract

Green ammonia has received increasing interest for its potential as an energy carrier in the international trade of renewable power. This paper considers Australia's prospects for green ammonia production from an exporter's perspective by highlighting Australia's competitive advantage in renewable resource quality and seasonal complementarity to its potential trade buyers. Although renewable resources are unevenly distributed across Australia and present distinct diurnal and seasonal variability, modelling shows that most of the pre-identified hydrogen hubs in each state and territory of Australia can produce cost-competitive green ammonia providing the electrolysis and Haber-Bosch processes are partially flexible to cope with the variability of renewables. Flexible operation reduces energy curtailment and leads to lower storage capacity requirements using batteries or hydrogen storage, which would otherwise increase system costs. In addition, an optimised combination of wind and solar can reduce the magnitude of storage required. Providing that a partially flexible Haber Bosch plant is commercially available, our modelling shows a levelised cost of ammonia (LCOA) of AU$756/tonne and AU$659/tonne in 2025 and 2030, respectively. Based on these results, green ammonia would be cost-competitive with grey hydrogen in 2030, given a feedstock natural gas price higher than AU$14/MBtu. For green ammonia to be cost-competitive with grey hydrogen, assuming a lower gas price of AU$6/MBtu, a carbon price would need to be in place of at least AU$123/tonne. A further factor favouring Australian production of green ammonia is the potential synergy between Southern Hemisphere supply and Northern Hemisphere demand. Given that there is a greater demand for energy in winter concurrent with lower solar power production, there may be opportunities for solar-based Southern Hemisphere suppliers to supply the major industrial regions, most of which are located in the Northern Hemisphere.

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Keywords: renewable/green hydrogen, ammonia, techno-economic modelling, energy storage

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Abbreviations	
AE	Alkaline electrolysis
AEMO	Australian Energy Market Operator
BESS	Battery energy storage system
CAPEX	Capital expenditure
COP26	2021 United Nations Climate Change Conference
HB	Haber-Bosch process
HEFT	Hydrogen Economic Fairways Tool
IRENA	International Renewable Energy Agency
LCOA	Levelised cost of ammonia
MIP	Mixed integer programming
MUREIL	Melbourne/Monash University Renewable Energy Integration Lab
NDCs	Nationally determined contributions
NSW	New South Wales
NT	Northern Territory
OPEX	Operational expenditure
PEM	Polymer electrolyte membrane
QLD	Queensland
RE	Renewable energy
SA	South Australia
SMR	Steam methane reforming
SOEC	Solid oxide electrolyzer cell
TAS	Tasmania
VIC	Victoria
WA	Western Australia
WACC	Weighted average cost of capital

Nomenclature

1. Introduction and Background

Despite the nationally determined contributions (NDCs) committed to before the 2021 United Nations Climate Change Conference (COP26), global warming will likely exceed 1.5 degree Celsius during the 21st century [1]. A more urgent and rapid acceleration of mitigation efforts is required to achieve global net-zero CO2 emissions by 2050 [1, 2]. Hydrogen produced by renewable resources will likely play a key role in decarbonising the hard-to-abate sectors, such as fertilisers [3], steel manufacturing [4, 5], aviation [6], marine [7], and heavy-duty road transport [8, 9]. Due to local renewable energy resource limitations and land constraints, green hydrogen production might not be sustainable in major industrial countries, such as Germany [10] and Japan [11], who therefore intend to import hydrogen. Due to access to abundant renewable resources, a highly skilled workforce [12] and a politically stable environment [13], Australia is arguably well placed to participate in this international hydrogen-energy market. In November 2019, the Australian federal government launched its National Hydrogen Strategy [12] with the goal of positioning Australia as a major player by 2030. Several other studies have also recognized Australia's potential competitive advantage in the emerging hydrogen economy [14, 15, 16, 17, 13].

For long-distance delivery to international markets, hydrogen or energy carrier derivatives such as ammonia need to be compressed or liquefied. Of the potential energy carriers available, ammonia is perhaps the most promising. Shipping ammonia is commonplace today [18] as it is one of the world's most widely used chemicals. It has relatively high volumetric energy density (12.7 MJ/L) [19] and low storage pressure, as compared with other energy carriers such as liquid hydrogen (8.49 MJ/L) or compressed hydrogen (4.5 MJ/L) at pressure of 69 MPa and temperature of 25°C [19]. A recent study by IRENA [20] reviews the efficiency of different hydrogen carriers in the global trade to meet the 1.5 degree Celsius climate target. The reduced transport costs make ammonia ships the most appealing in terms of a broad variety of size and distance combinations in global commerce. This has also been illustrated by a study conducted by the Royal Society [18]. Likewise, a German-Australian joint research project [21] found that transporting ammonia 20,000 kilometres from Australia to Germany will be far less expensive (NH3: AU\$0.030 per tonne-km vs H2: AU\$0.090 tonne-km) and more technically feasible than previously assumed. A major concern with using ammonia as an energy carrier is that its re-conversion to hydrogen by cracking leads to an energy loss of 13-34% [22]. However, direct use of ammonia for existing purposes, like fertiliser production, or prospective applications, like bunkering fuel, avoids this energy loss and cost penalty [22].

Bilateral ammonia trade agreements and joint efforts in project development have started to emerge between countries and major international companies. The Japanese Ministry of Economy, Trade, and Industry [23] began promoting a new Road Map for Fuel Ammonia in early 2021. It focuses on co-burning ammonia in thermal power plants and use as a fuel for shipping. According to Stocks et al. [24], co-firing green ammonia produced in Australia in coal plants in Japan could reduce emissions by 43 Mt per year by 2030. Japan aims to import 3 million tonnes of green ammonia annually by 2030, and 30 million tonnes annually by 2050. In early 2022, Australia signed a bilateral hydrogen and ammonia trade agreement with Japan aiming to ship ammonia from Australia starting from the 2030s [25]. At the same time, new partnerships have also been formed with Australia's European counterparts. The Rocky Mountain Institute has released a new paper outlining a timeline for the EU to begin importing renewable energy in the form of hydrogen or ammonia as early as 2024 [26]. The report states imports of renewable ammonia would satisfy urgent industrial needs, radically altering the energy consumption profile of emission-intensive EU industry [26]. The promotion of a two-way trade between Australia and the EU has been supported by state governments and industries. The Queensland Government has signed a Memorandum of Understanding with the Port of Rotterdam to collaborate on opportunities to develop a hydrogen export supply chain [27]. In March 2022, Fortescue Future Industries and Germany's E.ON signed a major hydrogen supply and distribution deal [28]. By 2030, Fortescue aims to provide Europe with 5 million tonnes of green hydrogen per year, which will be distributed by E.ON [29].

The current international ammonia market, which is responsible for 1.3% of global CO2 emissions (450 Mt) [3], has an annual production capacity of around 175 million tonnes and a market value of approximately US$70 billion [30]. IRENA [31] projects global demand for ammonia to increase significantly to around 700 Mt/annum by 2050 in line with the 1.5°C scenario. Even to replace the current fossil-fuel ammonia would require 1750 TWh of renewable electricity (assuming 10 MWh per tonne ammonia) - which is around 7 times Australia's current annual electricity generation. It is therefore important to understand the key cost drivers and trade-offs between different system configurations for cost-optimal design before the roll-out of the industry.

As of 2022, in Australia, most green ammonia projects are either in pre-feasibility or pilot stage and are considered "pre-commercial". In the early phase of investments, developers are mainly blue-chip corporations or otherwise supported by governments through project funding. Early ammonia project implementation tends to favour grid connection with a renewable PPA. Grid-connected projects include GERI [32], QNP [33], DNM [34], H2TAS [35], H2U [36].

Meanwhile, large-scale, completely off-grid ammonia production systems targeting international export markets have become increasingly relevant in Australia, especially in remote locations without access to the major electricity grids. Those off-grid projects in development include the Asian Renewable Energy Hub (26 GW of wind and PV) [37], the Murchison PtX project (5.2 GW of wind and PV) [38] and the Western Green Energy Hub (50 GW of wind and PV) in Western Australia, as well as the Moolawatana Renewable Hydrogen Project (6 GW of wind and PV) [39] in South Australia. Successful conversion from concept to pilot scale to commercial operation depends on many factors, such as scale, location, access to existing infrastructure, PV vs. wind ratio, onsite storage, international shipping, and other financial factors.

Many techno-economic studies on green hydrogen have been undertaken [40], but only a handful are on green ammonia. Those ammonia studies examine the configurations of ammonia production systems that differ in terms of renewable generation technology, source of dispatchable power for balancing wind and solar, and the flexibility of the HB. [41] compares the economics of blue and green ammonia production in Europe. [42] studies a solar-PV generation system with battery and an inflexible HB for ammonia production in UAE, while [43] studies a wind powered ammonia productions for a remote island. [44] studied an ammonia production system powered by a hybrid wind-solar PV system with grid electricity for balance. [45] quantifies the benefit of flexible HB, which is powered by wind and solar PV with grid electricity for balance in Chile and Argentina. [46] also compare inflexible and flexible HB in solar PV and Concentrated Solar Power systems for ammonia export from Atacama Desert to Japan.

A few studies have undertaken a least-cost optimisation to estimate the levelised cost of ammonia. [47] focused on the potential for grid connection to lower the levelised cost of ammonia in Australia. They found that grid connection lowered the levelised cost of ammonia by reducing storage costs. However, a challenge with grid connection is the emission intensity can be comparable to conventional fossil fuel based ammonia production, even where the share of grid electricity is small [48]. [49] and [50] focused on the identification of global sites with the best solar and wind resources. They found that green ammonia could be produced at the best sites at a cost that is competitive with fossil-based ammonia by 2030, with substantial scope for up-scaling production.

The context for this paper is green ammonia for export, with estimations of seasonal production variability at key sites in Australia. Planning and decision making for a green ammonia export facility is dependent upon many factors. Generic costs can be captured in conventional levelised cost studies. However, many cost, and non-cost, factors are specific to plant location. Given that the availability of favourable wind and solar resources often occurs in remote locations, it is important to include region-specific factors where possible. Some of these include existing or planned infrastructure, roads, ports and industrial facilities. Remote location may preclude connection to a major grid. A further aspect is the potential complementarity of seasonal wind and/or solar with seasonal demand of potential buyers. Given that supply based on wind and/or solar is likely to be variable, the match, or mis-match, between supply and demand, and commensurate price variance, may be important determinants of economic viability.

While hydrogen and ammonia-related techno-economic feasibility studies have been undertaken, to our knowledge, there has been no dedicated study for an off-grid system that has quantified the benefits of Haber-Bosch (HB) operational flexibility with support of various storage duration. We address costs from a potential exporter's perspective, taking into account the availability of existing infrastructure. We also consider the complementarity of seasonal supply with seasonal demand for potential trade partners. We undertake a techno-economic assessment, encompassing the whole of Australia, to answer the following four questions:

1. Where are the locations for green ammonia project development in Australia that have the potential for lowest cost production, based on a target year of 2030?
2. What are the strategies for system optimisation and trade-offs between different generation configurations considering the operational flexibility of electrolysers and HB?
3. To what extent, could seasonal solar resource availability in Australia complement seasonal

demand in the Northern Hemisphere?

4. What are the corresponding cost-competitive (or break-even) carbon prices for key ammonia production sites?

In order to answer these questions, it is important to consider both the location related factors that influence potential viability, and the temporal availability of solar and wind resources. We assess location related factors with our Hydrogen Economic Fairway Tool (HEFT), developed in collaboration with Geoscience Australia [14]. The tool identifies regions across Australia with high potential for hydrogen production by considering renewable resource quality, access to water, ports, roads, railways, electrical transmission, and other existing critical infrastructure. We assess temporal availability with our "MUREIL-Ammonia" model, which is an extension of our MUREIL electricity capacity expansion model. "MUREIL-Ammonia" is a Mixed Integer Programming (MIP) model which allows a detailed temporal study of those high potential "hydrogen hubs" identified in the HEFT tool. MUREIL-Ammonia is developed as part of the Melbourne/Monash University Renewable Energy Integration Lab (MUREIL) - a capacity expansion and sector coupling model for Australian energy systems [17, 51]. MUREIL-Ammonia can evaluate the impact of temporal operational flexibility of electrolysers and the HB process with the support of various storage options and the electricity grid on the optimal design of the production system for hydrogen or ammonia at an hourly resolution. Drawing on the capabilities of HEFT and MURIEL-Ammonia, we analysed and compared the economic viability of potential green ammonia projects with various system configurations and calculated the associated Levelised Costs of Ammonia (LCOA) and fuel-switching carbon prices at the pre-identified hydrogen hubs in Australia.

This paper is structured as follows: Section 1 introduces the motivation behind this study and sets the four guiding questions for this paper and reviews the current techno-economic studies for green ammonia production and positions this study within the literature. Section 2 introduces the two models we used to identify the high-potential hydrogen hubs and further optimise the ammonia production system within these hubs. Model input assumptions are also discussed in Section 2. Section 3 discusses the modelling results. Section 4 concludes the paper and outlines the direction for future studies.

2. Model Description and Input Assumptions

2.1. Identifying potential hydrogen hubs

This paper first assesses the factors contributing to Australia's potential for green hydrogen production and identifies key regions of interest for this emerging industry. These regions are cross-referenced against areas of high potential for hydrogen production identified by Monash/Geoscience Australia's Hydrogen Economic Fairways Tool (HEFT).

The HEFT analysis accounts for both the quality of the renewable energy source, the availability of local infrastructure (road, rail, water and power) as well as plant economics when assessing the

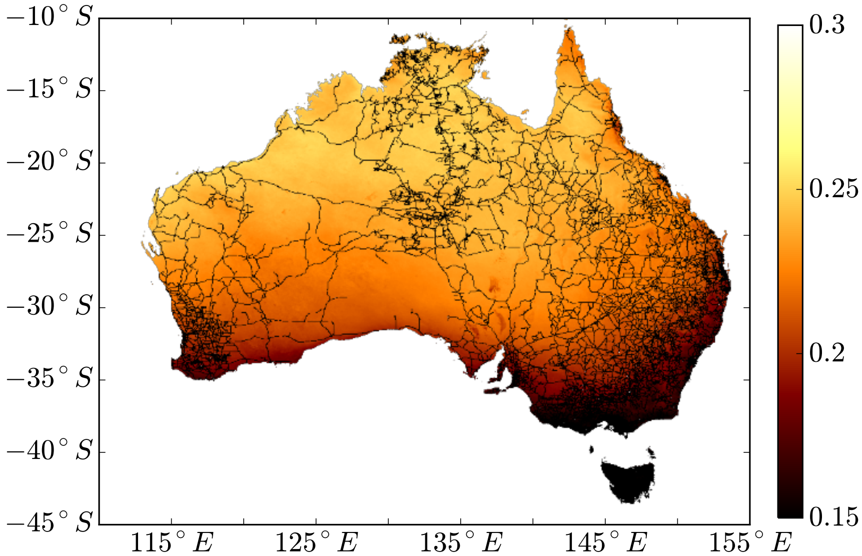

Figure 1: Transportation infrastructure map overlain with annual average solar capacity factor for Australia

Table 1: Identified 21 hydrogen hubs with quarterly (Q1-Q4) and annual average capacity factors for regional wind and solar resources.

State	Potential H2 Hubs		Solar Capacity Factor					Wind Capacity Factor				
			Q1	Q2	Q3	Q4	Annual	Q1	Q2	Q3	Q4	Annual
QLD	Q1	Far North QLD	20%	23%	27%	27%	24%	45%	51%	47%	38%	45%
	Q2	Townsville	22%	22%	27%	28%	25%	34%	36%	25%	26%	30%
	Q3	Julia Creek	26%	25%	28%	30%	27%	35%	50%	46%	40%	43%
	Q4	Gladstone	26%	22%	26%	28%	25%	41%	39%	25%	32%	34%
	Q5	Gibson Island	27%	22%	26%	30%	26%	33%	33%	33%	35%	34%
NSW	N1	Hunter	26%	18%	22%	27%	23%	22%	19%	30%	26%	24%
	N2	Southern Tablelands	26%	18%	21%	29%	24%	23%	25%	41%	35%	31%
VIC	V1	Gippsland	26%	16%	18%	29%	22%	24%	31%	42%	37%	34%
	V2	Geelong	28%	14%	16%	28%	22%	31%	45%	50%	41%	42%
	V3	Portland	26%	12%	14%	25%	19%	34%	47%	51%	48%	45%
SA	S1	Leigh Creek	30%	23%	26%	32%	28%	38%	37%	39%	45%	40%
	S2	Eye Peninsula	30%	19%	22%	32%	26%	36%	37%	39%	42%	39%
TAS	T1	North West TAS	26%	11%	12%	25%	19%	40%	42%	47%	45%	43%
	T2	Bell Bay	29%	14%	16%	30%	22%	35%	39%	46%	42%	41%
WA	W1	Pilbara	24%	25%	28%	30%	27%	26%	32%	32%	31%	30%
	W2	Geraldton	30%	21%	25%	32%	27%	52%	44%	38%	50%	46%
	W3	Kwinana	31%	19%	21%	32%	25%	44%	42%	35%	45%	42%
	W4	Kalgoorlie-Boulder	30%	22%	24%	32%	27%	42%	42%	40%	42%	41%
NT	NT1	Darwin	14%	24%	27%	21%	21%	27%	27%	19%	8%	20%
	NT2	Baines	20%	25%	28%	24%	24%	21%	47%	46%	24%	35%
	NT3	Tennant Creek	28%	27%	30%	29%	28%	42%	54%	54%	43%	48%

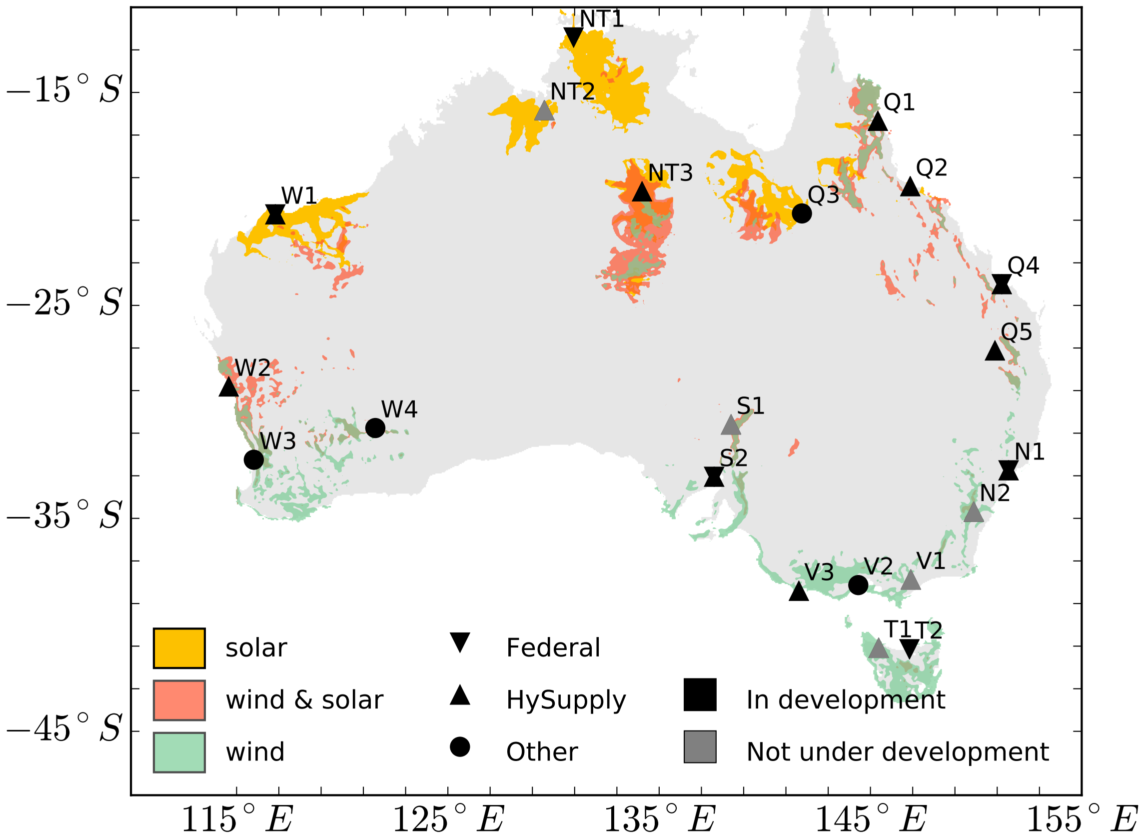

Figure 2: High potential regions (ranked in the 95th percentile) for the production of farm-gate and off-grid hydrogen from solar, wind and hybrid (wind & solar) sources. Locations labeled on the map indicate the position of key hydrogen hubs considered in this paper.

potential for hydrogen production [14]. An example of the infrastructure map with annual average solar capacity factors is shown in Figure 1. Details of the HEFT model can be found from [14].

We consider three different configurations of renewable energy - solar only, wind only and a hybrid system with 50% wind and solar power. From this analysis, we identified those regions in the 95^{th} percentile for hydrogen production from each of the three power source variations considered. These are indicated by the coloured regions in Figure 2. These regions were then cross checked against the locations of major hydrogen hubs or high-potential locations proposed by either the Federal government's hydrogen initiative [52], the independent HySupply study [53], or suggested as part of industry projects.

The resulting 21 locations were then selected for more detailed site-based studies. Those locations include Q1-5 from Queensland (QLD), N1-2 from New South Wales (NSW), V1-3 from Victoria (VIC), S1-2 from South Australia (SA), W1-4 from Western Australia (WA) and NT1-3 from the Northern Territory (NT). Most of the highlighted hydrogen hubs are located near the coast with the exception of Q3, S1, NT3 and W4. Names of all the hubs along with their renewable resource potential are shown in Table 1. Hydrogen projects in development [54] within these locations are also indicated in Figure 2. With these high potential hubs being identified, we then use the MUREIL-Ammonia model to find the optimal plant configuration for each of them, as described in the following sections.

2.2. Schematic of the off-grid ammonia production system

In the early 1900s, Fritz Haber devised a method of fixing nitrogen by combining atmospheric nitrogen and hydrogen in the presence of a metal catalyst to produce ammonia, commonly known as the Haber-Bosch pathway (HB). Although process technology has improved over the years, the basic chemistry is identical to the original process developed [55]:

$$N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)\Delta H = -92kJ/mole\,(-46kJ/mole\ for\ 1\ mole\ of\ NH_3)$$

There are multiple pathways for producing feed hydrogen and nitrogen for HB, but the most common method at present is via reforming of natural gas, and cryogenic air separation of nitrogen [56]. In this pathway, CO_2 is generated as a product of the reforming process and through the combustion of natural gas for process heat. The reform process produces a concentrated stream of CO_2, which can be captured and stored, whereas the combustion process produces a dilute stream of CO_2, which is less easily captured. If most of the CO2 is captured and sequestered, the ammonia may be termed 'blue'. If the CO_2 is released to the atmosphere, the ammonia is termed 'brown'. So-called 'green' ammonia is also produced with the HB process, except that the hydrogen feed is sourced via renewable energy. There are several means to produce green hydrogen, but the approach that is envisaged to be the most scalable and cost effective in the long term is water electrolysis powered by wind and/or solar electricity. Energy demand for cryogenic air separation of nitrogen is relatively small compared to the requirements for hydrogen production, and is also sourced from renewables for green ammonia. In the longer term, direct electrochemical reduction of nitrogen may offer the potential for modular devices that overcome the limitations of HB (e.g., [57, 30]). Such devices could potentially offer greater operational flexibility, and therefore synergistic integration with renewable energy. However, these potential advances are not considered in this modelling study.

In this study, we focus on the HB process, as a mature technology, for ammonia production modelling. The HB ammonia synthesis loop comprises a synthesis reactor, mixing units, compressors, heat exchangers, and an ammonia separation unit. The feedstocks are hydrogen from the electrolysis units, and nitrogen from the air separation unit. The reactor operates with a pressure of typically 150 to 300 bar and a temperature of 350 to 550 °C. The reactor conditions are designed to achieve a sufficiently high reaction rate since the yield per single pass is typically only around 15 to 25%. The catalyst type, feed content and composition also influence the operation. Given the multiple constraints on operation, synthesis loops are typically optimised for steady state operation at near full capacity with limited capability for reduced operation. Figure 3 shows the schematic of the off-grid version of the MUREIL-Ammonia model with various buffering mechnisums to achieve continuous operation. As illustrated in Figure 3, off-grid electricity for powering hydrogen electrolysers, the air separation unit and the HB process for ammonia production can be supplied by the onsite wind, PV or a hybrid system consisting of wind and PV. This system may be supported by an onsite battery with 2, 4 and/or 8-hours of storage and hydrogen storage tanks as buffering mechanisms. Battery storage is better suited for balancing hourly and daily variations of RE to meet the operational requirements of the entire system, whereas H2 buffer/storage tanks are required primarily for balancing RE variations at the seasonal or synoptic timescales to meet the operational constraints of the HB system. Cost-optimal designs are calculated among these generation and storage options to produce ammonia at an average output of 100 tonnes daily, which is considered to be a small-to-medium project size starting from 2025. We set an annual production volume of 36,500 tonnes, with an additional 5% to account for periodic maintenance. We did not set daily production as a constraint so as to explore the impact of hydrogen storage capacity in response to seasonal variability of renewable resources. Sizing of ammonia storage is intentionally omitted because it is a non-optimisation variable and we did not specify a schedule for ammonia off-take. Future studies will factor in ammonia storage as an optimisation variable when imposing different temporal production/delivery commitments (e.g., weekly, monthly or quarterly) dictated by potential off-take agreements. Model input assumptions are discussed in detail in the following sections.

2.3. Modelling system flexibility

Matching variable electricity supply with electrolysis and HB is a significant challenge. Of the available electrolyser technologies, proton exchange membrane (PEM) electrolysers possess the highest operational flexibility and turndown capability. However, PEM is currently more expensive than alkaline electrolysers (AE) [58]. Depending on make and model, AE generally possess less

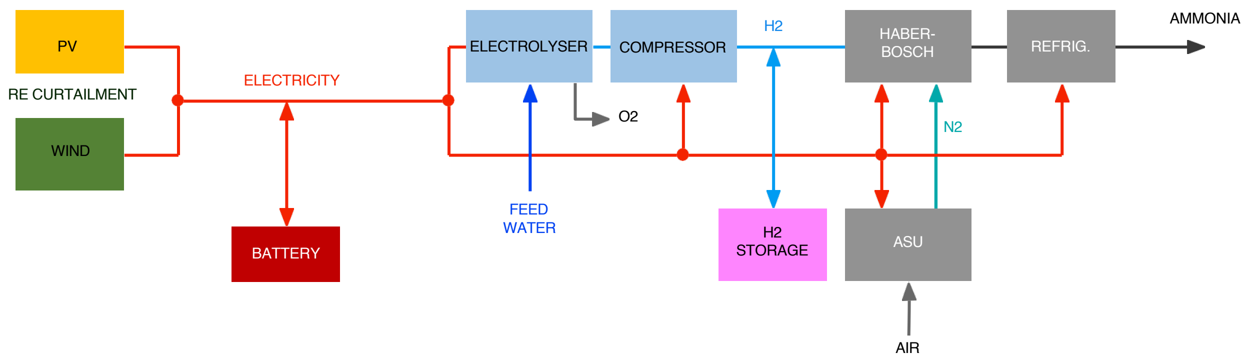

Figure 3: Schematic of major components considered in the off-grid green ammonia production model

operational flexibility, but can usually be operated dynamically, albeit with a higher minimum load. Some models can be placed into a warm standby condition, and it is also possible to regularly shut down a stack without serious degradation of catalysts. A further factor is that the modularity of electrolyser stacks opens the possibility for dynamically controlling banks of stacks to achieve system-wide dynamic operation. It may be feasible, for example, to shut down a bank of stacks during winter as a strategy for optimising usage in response to low solar conditions. For these reasons, we chose AE for the techno-economic modelling given the target time horizon of 2025 to 2030. We assume the overall system turn down ratio is 80% of the installed capacity (i.e., 20% minimum stable generation needs to be maintained in operation) and a moderate hourly ramping constraint of 40% of installed capacity. Sensitivity of key AE operational parameters on LCOA is illustrated in Figure 8 and is discussed in detail later.

The greater challenge for ammonia production is reducing load variability within the ammonia synthesis loop [59]. As noted earlier, the reactor environment of ammonia synthesis constrains the capability of dynamic operation, necessitating nearly continuous feed of hydrogen, nitrogen, and process electricity. The high thermal inertia and high operating pressures of some processes reduce permissible ramp rates, and preclude frequent start-ups and shut-downs. Some components, such as compressors, pumps and chillers units, are typically optimised for steady state operation within a prescribed operating envelope, although the envelope is usually wide enough to provide for some flexibility. The turndown of synthesis loops is conventionally limited to 40% (i.e., minimum operation of 60%) and a dynamic ramp rate of 20 % per hour. These operational parameters found in the literature are used for for this study [45]. Sensitivity on HB operational parameter assumptions are also studied.

2.4. Partial load efficiency

The varying load efficiency of key components of the ammonia production system is an important feature to be included in the modelling. The energy efficiency of AE electrolytic cells is lower at

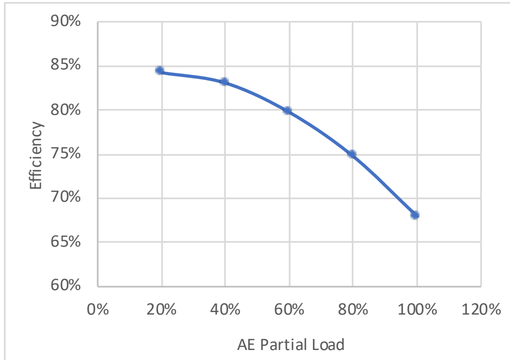

Figure 4: AE partial load efficiency gain [53, 61]

high current load due to declining voltage efficiency at higher current density. This is mainly a result of ohmic resistances, and reactant and product diffusion to and from the electrodes. For the AE we applied the generic load-efficiency transfer function shown in Figure 4.

Unlike AE, the energy efficiency of HB is likely higher at full load, with a decline at partial load. However due to a lack of publicly available data we do not model efficiency as a function of load, instead applying a constant efficiency shown in Table 2. Since the HB reaction is exothermic, we assume that the output chemical energy flux of NH3 is 88% of the input energy flux from H2 [45].

AE must be operated above a minimum load, which is typically 10 to 40%. Below the minimum load, gas diffusion across the membrane causes a rise in gas impurity in both the hydrogen and oxygen streams. Hydrogen contamination in the oxygen stream, even at relatively low levels, results in a flammable mixture. Commercial units incorporate safety systems that activate at a hydrogen contamination of 1 to 2% in the oxygen stream [60].

According to [45], when the HB loop's load varies from nominal, its efficiency will likely decrease. To account for this, we also adopted the approach from [45] that use estimates of the HB-power ASU's consumption of a 20% constant component (0.64 MWh/t NH3) and a variable component proportional to the reactor's hydrogen intake flow. This modelling is imprecise, but an HB machine's electricity use is only a small component of LCOA [45].

2.5. Modelling of storage systems

Solutions to maintaining high utilisation of the production plants with onsite renewables involve both short and long term storage. As the synthesis reaction is exothermic, most of the energy requirement is for hydrogen production, and consequently, large-scale buffering of the gaseous hydrogen feed is one strategy to increase utilization. Reported costs for hydrogen tank storage range from 280 to 2100 AUD/kg depending on size and pressure [45, 62], with the mid-range of current prices reported at around 700 AUD/kg and ambitious long-term goals of 110 AUD/kg [45, 62]. We assume hydrogen storage in 2030 at AU$60/kg (AU$18/kWh), which is in line with [45, 62] for this study, with a cost sensitivity analysis conducted in Figure 8. It is noted that in energy terms, hydrogen storage is far less costly than battery storage (AU$500/kWh [58]) and more expensive than ammonia storage AU$0.2/kWh [45, 62]. According to Geoscience Australia [54], the Pilbara (H2 hub W1) has access to underground salt cavern storage, which could be much cheaper than pressurised tanks for large-scale hydrogen storage. For consistency, we did not include salt cavern storage in this study, but will look into it in future studies.

Another strategy is electricity buffering via battery storage or via grid firming. Regardless of buffering strategy, some form of electricity storage or back up power will be required to maintain standby operation, safety systems and controls. Battery storage is needed for an off-grid system to not only balance RE to meet the operational requirements of the AE, but also power the ACU, HB and other auxiliary systems when RE is unavailable. As BESS is one of the system's most expensive components, we modelled BESS with 2, 4 and 8 hours of storage duration as separate units. This practice allows the optimisation to choose the best option that suits the unique characteristics of the renewables onsite.

Future, possibly small scale, Haber Bosch systems may be optimised for dynamic operation, and open opportunities for integration with renewable energy with less requirement for buffering or large scale storage. We study this by varying the maximum turn-down ratio and ramping constraints in the sensitivity study.

2.6. Modelling of RE generation

The average annual wind and solar capacity factors in 2019, which indicate renewable resources quality for these hydrogen hubs are shown in Table 1. Hourly wind and solar capacity factor time series for the identified locations are taken from the Renewables.Ninja database [63, 64]. Onshore wind turbine (Vestas V80 2000) with a hub height of 150 m and solar PV with one axis tracking are specified when retrieving the data.

2.7. Technology cost assumptions

Technology costs are also essential assumptions in any techno-economic models. Where possible, we tend to use technology cost projections from Australian reports that better reflect Australian contexts as an exporter. Most of the key technology CAPEX and OPEX are taken from the Australian Energy Market Operator (AEMO) Integrated System Plan 2022 [65] Inputs and Assumptions Workbook and are summarised in Table 2. Most of the facilities are assumed to have an economic life of 25 years, whereas BESS is assumed to have a lifetime of 15 years, and AE lifetime is assumed to be 80,000 hours of operation. Sensitivity on the key CAPEX components is conducted in Figure 8.

The weighted average cost of capital (WACC) is assumed to be 7.5%, which lies at the upper bound of that used in the 2022 Integrated System Plan (ISP) [65] by AEMO. Sensitivity of WACC on LCOA is conducted in Figure 8.

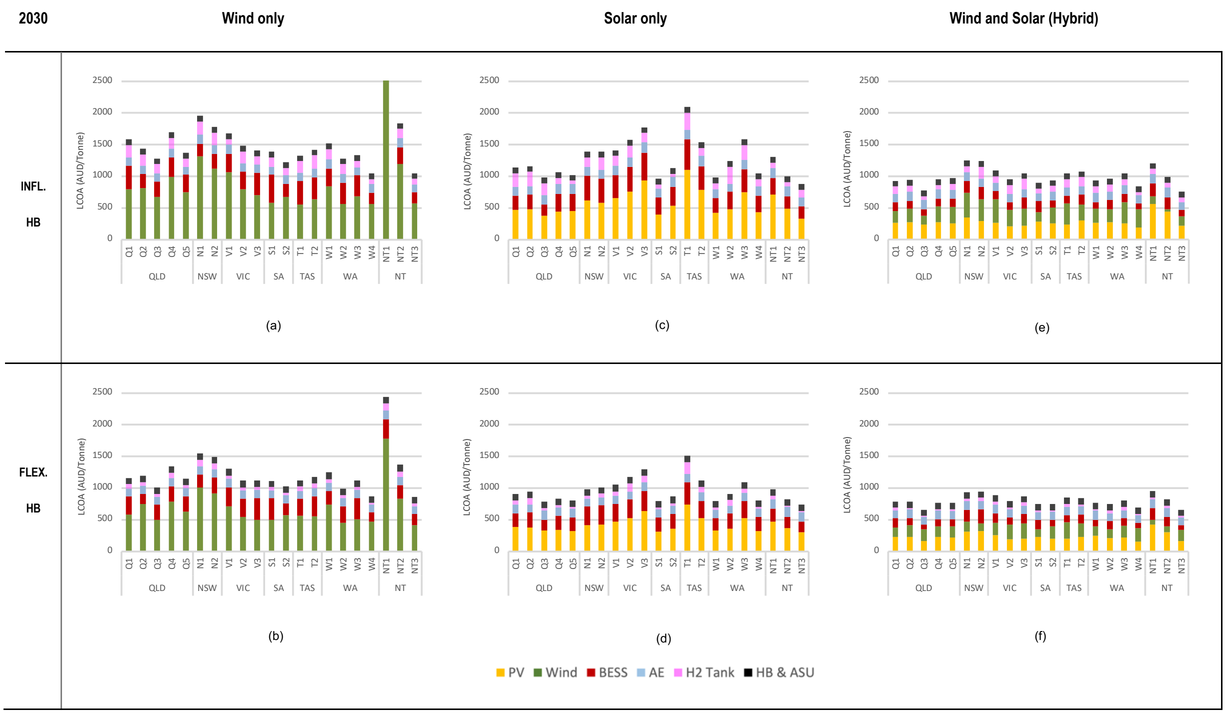

Figure 5: Levelized costs of Ammonia (LCOA) using 2030 CAPEX assumptions for scenarios with wind only, solar PV only and a hybrid wind and solar system

2.8. Model implementation

MUREIL-ammonia is a mixed-integer program. Electrolyser partial load efficiency is implemented by introducing piecewise-linear constraints. Minimum cold-stop duration is also modelled with binary variables. However, to reduce computational complexity, this constraint is not activated if the system is only allowed for partial flexibility. Wind, PV, AE, ASU, HB, BESS, and hydrogen tank capacities are modelled as continuous variables for computational manageability. In real-world project implementation, those components might have a standard unit size depending on the vendor and availability in the market. In this case, the number of units needs to be modelled with integer variables. In this study, we assume a generic model that can be optimally sized at any capacity.

3. Results and Discussion

3.1. Levelised cost of ammonia

Here we compare the results from wind only, solar PV only and hybrid wind-solar systems with flexible and inflexible HB processes. The levelised cost of ammonia (LCOA) for inflexible

Table 2: Key cost assumptions employed in the MUREIL-Ammonia Model.

Component	Project Start 2025 *	Project Start 2030*
Alkaline electrolysers (AE 68-84% eff. LHV [53, 61])	\$808 /kW	\$485 /kW † [58]
- Min Stable Generation: 20% of installed capacity [66]; Stack lifetime: 80000 hours [66]		
Wind	\$1939 /kW	\$1848 /kW ‡ [65]
Solar PV	\$906 /kW	\$796 /kW ‡ [65]
Battery Energy Storage System (BESS 2h 85% round-trip-eff.)	\$716 /kW	\$548 /kW ‡ [65]
Battery Energy Storage System (BESS 4h 85% round-trip-eff.)	\$1037 /kW	\$759 /kW ‡ [65]
Battery Energy Storage System (BESS 8h 85% round-trip-eff.)	\$1717 /kW	\$1211 /kW ‡ [65]
H2 storage/buffer tank	\$600/kg H2 (\$18 /kWh) [45]	
Haber-Bosch plant (HB eff. 80%)	\$1,085/t/annum (\$850/kW) § ¶ [45]	
Air separation unit (ASU eff. 80%)	\$274/t N2/annum (\$382/kW) § [45]	
Elec. HB-ASU (MWh/t NH3)	0.64 MWh/tonne NH3 [45]	
Elec. pre-compression	0.26 MWh/tonne NH3 [45]	
Maximum turn-down ratio of AE	80% installed capacity [66]	
Maximum turn-down ratio of HB	40% installed capacity [45]	
max ramp	(+/- 20% load/h) [45]	
cold stop min. duration	48h [45]	
cold stop load	0 [45]	
Fixed OPEX of AE	3% of CAPEX/year [65]	
Fixed OPEX of HB, ASU	2% of CAPEX/year [45]	
Fixed OPEX of H2 tank	1% of CAPEX/year [45]	
Wind Fixed OPEX	\$28/kW/year [65]	
Solar Fixed OPEX	\$19/kW/year [65]	
BESS 2h Fixed OPEX	\$12/kW/year [65]	
BESS 4h Fixed OPEX	\$19/kW/year [65]	
BESS 8h Fixed OPEX	\$31/kW/year [65]	

*All costs AUD. Costs adjusted to 2021 AUD.
†based on the 2050 Global Net-Zero Emissions scenario from [58]
‡based on the Step Change scenario from [65]
§LHV H2 in [45]
¶\$/t/annum based on conversion efficiency 10.4 MWh/t and 93% utilisation rate

and flexible HB processes with different generation options are presented in Figure 5. The figure presents the contributions of the different components to the total cost. In general, modelling results indicate that all states can produce cost-competitive green ammonia if the system is flexible and optimally designed. Systems with a single generation source and inflexible HB are significantly more expensive.

With a single generation source (i.e., wind or solar PV-only), inflexible HB (Figure 5a, c and e) requires extensive buffering mechanisms and overcapacity of generation plants resulting in high system costs. In that case, only a handful of hydrogen hubs could produce ammonia at a cost close to AU$1000/tonne by 2030 from wind-only (Figure 5 a) or solar-only (Figure 5 c) powered systems. Significant oversizing of generation capacity to meet the annual production target is inevitable if the onsite wind or solar resource is of inferior quality. Sizable BESS and H2 tank storage are also required to balance daily and seasonal variations of the wind or solar generation plant. Inland hydrogen hubs (e.g., Q3, NT3), where solar resources present less seasonal variation, tend to perform better than coastal hubs.

Nevertheless, optimisation results show (Figure 5e) that if renewable electricity can be sourced from both wind and solar PV simultaneously (i.e., with a hybrid wind-solar PV generation system), the LCOA from coastal hydrogen hubs could be reduced by an average of almost 30% (37% compared to wind-only, 22% to solar PV-only) in 2030, achieving an average LCOA of $1000/tonne. This considerable cost reduction is because a well-mixed wind and solar PV system could improve electrolysis and HB capacity factors and significantly reduce the required RE capacity (and RE curtailment) and the need for BESS and hydrogen buffer tanks. Combining wind and solar to form a hybrid generation system is essential for cost reduction.

Equally important, the flexibility of HB (Figure 5b, d and f), especially with the partially relaxed minimum operational load requirement, is also key to facilitating large-scale ammonia production. Electricity generation and storage systems constitute the major components in the LCOA. Modelling results show the use of H_2 buffer tanks becomes minimal, with flexible HB for both the wind-only (Figure 5b) and solar PV-only (Figure 5d) powered systems. The use of batteries is also moderately reduced. In this case, most hydrogen hubs with a single RE generation source can produce ammonia at an average LCOA of AU$960/tonne for solar (compared to $1270/tonne from its inflexible counterpart) and AU$1200/tonne for wind (compared to $1550 from its inflexible counterpart) in 2030. Compared with inflexible HB for most cases, flexible HB reduces wind deployment in the optimal generation mix. A well-mixed wind and solar PV configuration further reduces the levelised cost of ammonia, which leads to LCOA being as low as AU$760/tonne in 2025 and AU$660/tonne (Figure 5 f) in 2030 at the most competitive hydrogen hubs.

We use modelling results for the Pilbara (location W1) to demonstrate the temporal evolution of system operation and highlight the benefit of flexible HB in the hybrid RE system. The Pilbara has one of the world's largest natural gas fertilizer production facilities with well-established ports and shipping infrastructure. Figure 6 shows one day out of the full year of modelled hourly interplay between the hybrid wind-solar PV generation system, BESS, hydrogen tanks, and the inflexible HB plant (Figure 6a) and the flexible HB plant (Figure 6b) at the Pilbara on the 12th of June in 2030 (using historical data from 2019). From Figure 6, solar PV dominates over wind for the Pilbara. Generally, any system with a large solar PV system needs BESS for continuous operation at night. Even a flexible HB still requires a considerable BESS to balance AE (to meet the AE's minimum operational load requirement) for hydrogen production as well as the ASU-HB system for ammonia production at night. Although the benefit of flexible HB in reducing the need for BESS in the hybrid RE system is moderate, partially flexible HB can reduce renewable curtailment and the size of the H2 tank significantly. This is further illustrated in Figure 7, which shows the monthly average RE curtailment and the average state of charge of the H2 tank throughout the year. For the partially flexible HB case, significantly less H2 storage is required, and the amount of wind and solar that is curtailed is much less.

By 2030, the LCOA of solar-powered ammonia is very close to that of the hybrid system because the CAPEX of solar PV is expected to reduce considerably.

Putting all these into context: in the best-case scenario, if Burrup Peninsula in the Pilbara was to replace 100% of its current natural gas ammonia (0.85 Mt/annum [67]) with green ammonia by 2030, it would at least require 604 MW of wind, 2140 MW of solar PV, 522 MW of 8-hour battery, 12 GWh of hydrogen tank storage, and 1188 MW of AE electrolysers and 700 MW of ASU-HB. The resulting LCOA from this hybrid system would be around AUD$ 768/tonne NH3 in 2030.

A sensitivity analysis was conducted on key input parameters, including the discount rate, plant CAPEX, and the operational specifications of the individual system components. Figure 8 shows the change in LCOA by varying the input parameter by +/-25%. From Figure 8, the discount rate has the greatest influence, overall, on the cost of green ammonia in 2030. These results might not be too surprising, since making green and ammonia both have high start-up costs and lengthy development periods. But this result does show how government policies, like low-interest loans and other ways to reduce the risk of investing in green ammonia, could help this emerging industry to take shape. The CAPEX of wind and solar PV is also very influential when the system is powered by a single generation source. Hybridization reduces the impact of individual generation technologies on total system costs as there is greater flexibility in the generation mix.

Sensitivity analysis also highlights the importance of HB flexibility on the overall system design. Results show the minimum operational load requirement of the HB has a greater impact than its CAPEX on total system costs as its minimum load requirement affects the sizing of other system components. The impact of the HB minimum load requirement is further intensified if the local RE resource presents strong seasonal variations, especially in solar-powered systems. In contrast, hourly HB ramping constraints have minimal effect on system design. On that note, research and development should perhaps focus on reducing HB minimum load requirements. AE minimum load requirements tend to affect wind-only installations more than other generation configurations, while BESS CAPEX tends to influence solar PV-only installations more. Overall, the change of CAPEX

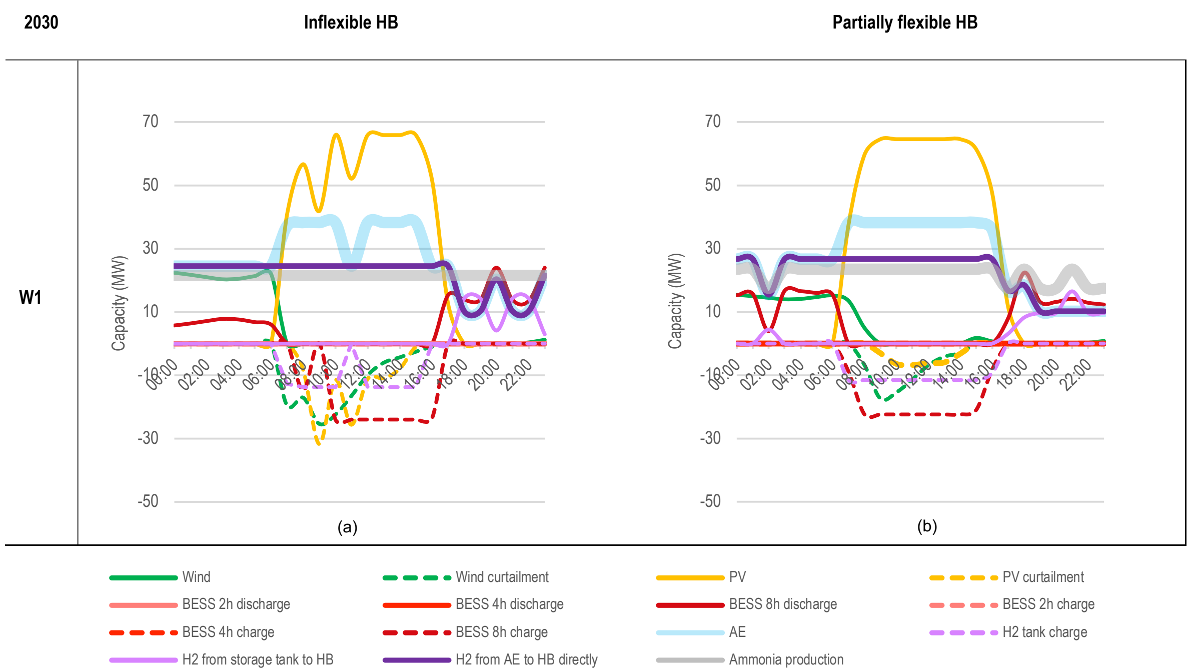

Figure 6: 12 June 2019 W1 Optimised capacity and hourly operation of the off-grid ammonia production system in the Pilbara region of Western Australia (W1) for the combined solar PV, wind and BESS scenario. Inflexibile HB (a), partially flexible HB(b)

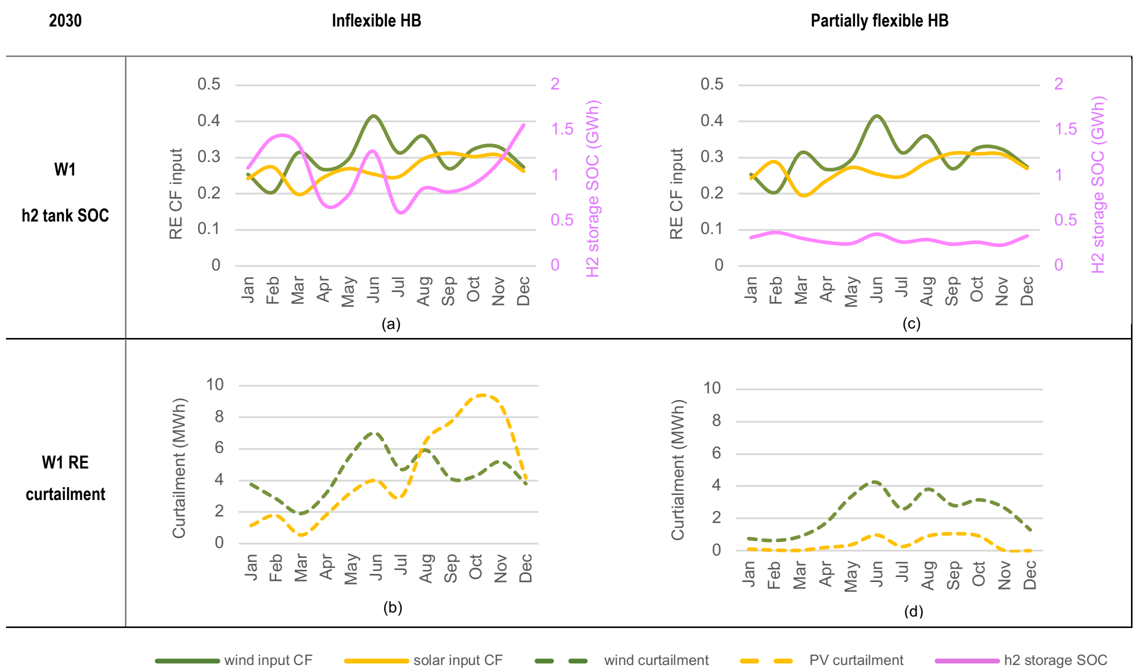

Figure 7: (a) and (c) Monthly average hydrogen tank SOC and input CF for wind and solar. (b) and (d) monthly average RE curtailed energy. Inflexibile HB (left), partially flexible HB (right)

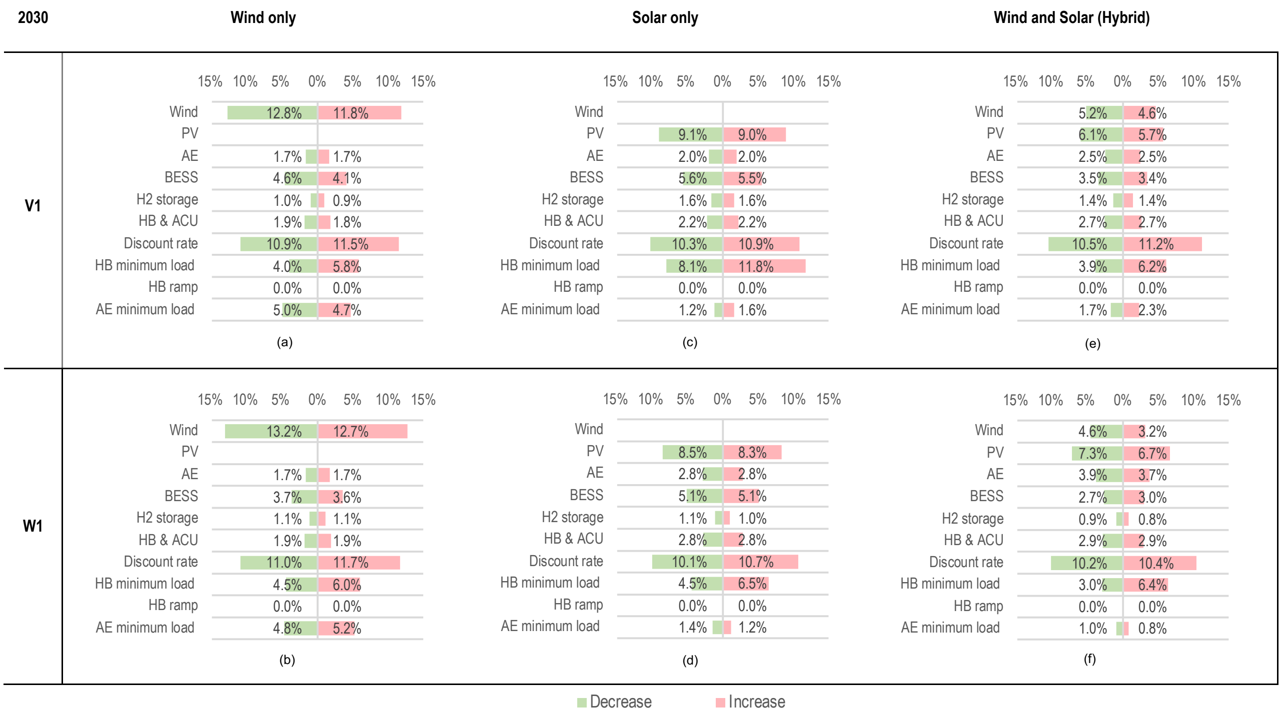

Figure 8: Sensitivity (+/- 25% of the baseline assumptions in Table 2) on key CAPEX assumptions in 2030, discount rate and plant flexibility specification for scenarios with wind only, solar PV only and the hybrid wind and solar system

in AE, BESS, and H2 tank has a moderate impact on total system costs. A similar situation applies to the HB and ACU components.

3.2. Break-even natural gas and carbon prices

To place these estimates in context we now compare the LCOA for hybrid wind-solar systems in 2025 and 2030 located in the Pilbara and Tennant Creek to the LCOA using Steam Methane Reforming (SMR). Using modelling from the IEA Ammonia Technology Roadmap [3] we estimated the SMR LCOA for difference combinations of the cost of natural gas and carbon prices, which are presented in Figure 9. This provides a map of the potential break-even points for green ammonia production in Australia, which are shown by overlaying lines and points that illustrate the combinations of natural gas and carbon prices that coincide with cost-parity between grey and green ammonia production.

Point a in Figure 9 shows the 2021 Tampa ammonia price in June 2021. We use an example price from 2021 as it was before the large increases in ammonia prices seen during 2022, which were as high as AU$1600/tonne [68]. When comparing the LCOA across types of production, the IEA [3] used AU$158 to AU$707/tonne as the range of average monthly ammonia prices for 2010-2020, which was based on US Gulf, Middle East and Western Europe spot prices.

Points b and c in Figure 9 shows the break-even points for green ammonia produced at Tennant Creek and the Pilbara in 2030 without a carbon price. This would occur with a cost of gas of AU$13.56/MBtu and AU$17.20/MBtu, respectively. If we assume a cost of gas of AU$6/MBtu, then cost-parity with ammonia produced via SMR would occur with a carbon price of AU$123/tonne and AU$183/tonne, respectively. These are shown in Figure 9 at points d and e. Additional comparisons can be made for different levels of gas costs by following the green and yellow lines. These carbon prices can also be referred to as cost-competitive carbon prices, which set the costs of grey and green ammonia supply equal.

3.3. Impact of seasonality on value of ammonia exports

So far in this paper we have compared LCOA for different generation configurations and estimated the corresponding fuel-switching carbon prices from ammonia produced in Australia. A critical aspect that has not been discussed is the end-use of hydrogen and its value, particularly to the potential importers. IRENA [20] projects 12% of the final global energy demand will be supplied by hydrogen in the 1.5°C scenario by 2050, with three-quarters of the hydrogen produced using domestic resources, leaving the remaining one quarter (150 Mt/annum) through international trade. Learning from experience in domestic reserves for oil and gas, we could shed light on the seasonally varying value of Australian hydrogen and ammonia exports to the major industrial countries in the Northern Hemisphere by comparing the importer's own seasonal production profile and energy consumption patterns throughout the year. The temporal gap between domestic supply and consumption would indicate the time of shortage and highlight the economic value of international imports at that particular time.

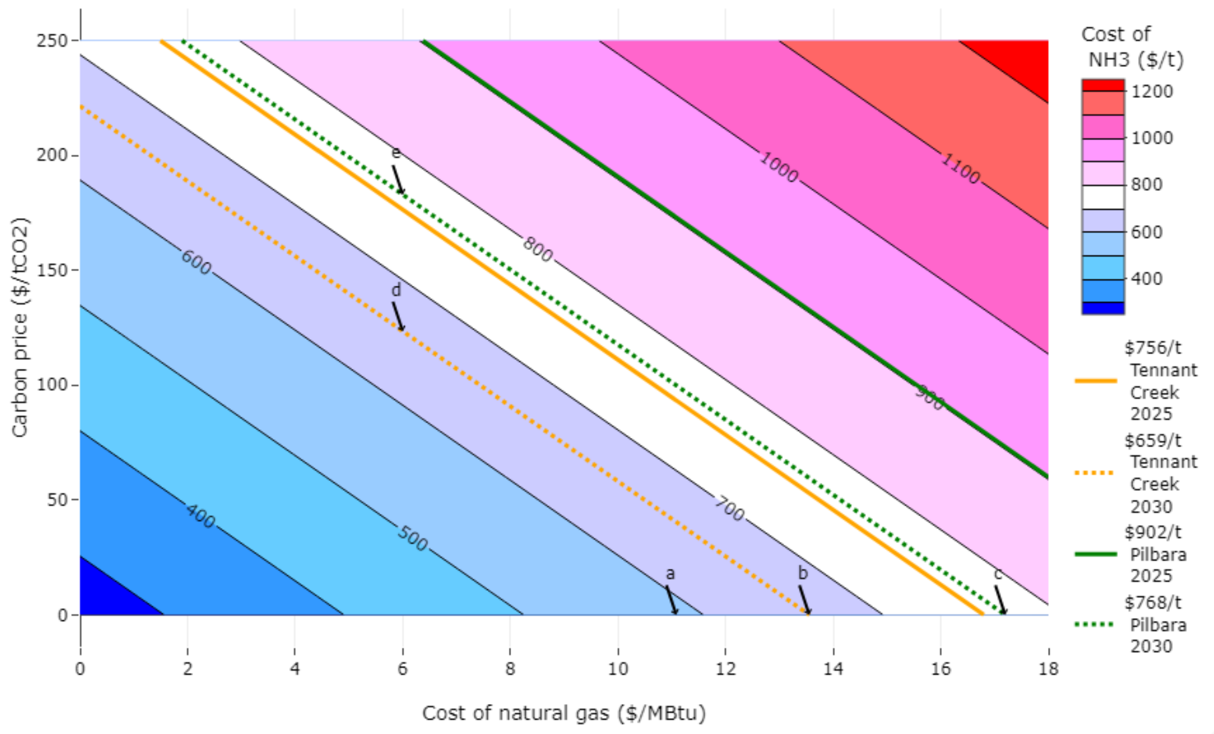

Figure 9: LCOA from Steam Methane Reforming (SMR) as a function of the cost of natural gas and carbon price. Estimated using a regression where LCOA = 253.22 + (29.93*cost of gas) + (1.83*carbon price) with a model fit of R-squared=0.99. Provides a comparison to the LCOA for hybrid wind-solar systems in 2025 and 2030 located in the Pilbara (green lines) and Tennant Creek (yellow lines). Arrows indicate the 2021 Tampa ammonia price without a carbon price (a), break-even point for Tennant Creek in 2030 without a carbon price [i.e., cost of gas at AU$13.56/MBtu] (b), break-even point for the Pilbara in 2030 without a carbon price [i.e., cost of gas at AU$17.20/MBtu] (c), break-even point for Tennant Creek in 2030 with the cost of gas at AU$6/MBtu [i.e., carbon price of AU$123/tonne] (d), break-even point for the Pilbara in 2030 with the cost of gas at AU$6/MBtu [i.e., carbon price of AU$183/tonne] (e).

Figure 10: (a) shows the seasonal anomaly relative to annual mean daily coal, oil, and gas CO2 emissions in China, the USA, the EU, and the globe as a whole from 1959 to 2018 [69]. It highlights that the seasonal use of fossil fuel peaks during the Northern Hemisphere winter. (b) Monthly solar PV capacity factor with one axis tracking in 2019 [63, 64] in selected industrial countries (c) Modelled optimal ammonia production profiles in NT3 from the wind only, solar PV only and the hybrid system across the year. (d) Modelled optimal ammonia production profile from solar PV in V1 shows strong seasonal pattern due to seasonality of solar irradiation. The hybrid wind-solar PV system can reduce seasonal variation.

Figure 10 (a) shows the seasonal anomaly relative to annual mean daily coal, oil, and gas emissions in China, the USA, the EU, and the globe as a whole from 1959 to 2018 [69]. It shows countries in the Northern Hemisphere have peak demand for coal, oil, and gas in the boreal winter (November to February) and reach their lowest demand in the boreal summer (June to September). The future use of hydrogen and hydrogen derivatives is also likely to peak in the winter of the Northern Hemisphere. The seasonal peak of coal, gas, and oil consumption in major industrial countries in the Northern Hemisphere is likely to indicate the potential demand surge of hydrogen and ammonia as a blending or substitutional fuel in the boreal winter, even to replace a small portion of the incumbent fossil fuel use for decarbonisation purposes.

In contrast to the seasonality of fuel demand, the potential domestic supply of green hydrogen and hydrogen derivatives from solar PV also presents a strong seasonal variation in the major industrial countries in the Northern Hemisphere. Figure 10 (b) shows the average monthly capacity factors for a single axis tracking PV system in the representative industrial zones in Germany, Japan, South Korea, China, and the USA, where solar PV generation peaks in the boreal summer and decreases significantly in the winter. The solar generation shortfall implies a substantial hydrogen supply deficit in the boreal winter using regional resources; however, this is when energy demand reaches its highest. The demand side would need to compete for the limited renewable generation resources in winter, which will likely drive up energy commodity prices, including green hydrogen.

The significant mismatch of demand and supply highlights the value of international exports in the boreal winter. To meet the enlarged demand-supply gap in winter, domestic producers would need to oversize their systems to produce additional hydrogen or ammonia in summer to be stored for winter use. However, this will lead to the systems running at a lower capacity factor in winter as well as requiring additional seasonal storage, which will lead to higher production costs. Rather than investing in additional production capacity and storage, it might be more economical to ship Australia's solar-powered ammonia to the trading partners in the Northern Hemisphere in November, December, and January, when solar production in Australia reaches its highest while the importer demand peaks and local supply plummets in Northern Hemisphere. Seasonal complimentarity will create a win-win situation for the importer and the exporter on opposite sides of the globe. This could be facilitated by an off-take agreement that requires higher seasonal delivery.

To maximise the full potential of seasonality complementarity would require the HB system to be partially flexible. Figure 10 (d) shows that with an annual production target and a partially flexible HB (with a 40% turn-off ratio), the simulated optimal production profile from the solar-powered system in Gippsland (V1) Victoria sees substantial seasonal variation aligned with solar irradiation across the year. Such a project would be better suited with an off-take agreement that requires higher seasonal delivery. It could also take advantage of a future spot market when the price of green ammonia is likely higher in the boreal winter. On the other hand, the optimal production profile from the hybrid wind-solar system sees less monthly variation. Projects with well-mixed wind and solar would be better suited with an off-take agreement that requires a fixed amount of monthly delivery. Temporally fixed delivery also applies to places with renewables that present less seasonal variation, such as Tennant Creek (NT3) in the NT, as shown in Figure 10 (c).

4. Conclusion and Future Work

We have identified high potential hydrogen hubs considering regional renewable resources quality and critical infrastructure for the whole of Australia and then used a Mixed Integer Programming model to conduct a more detailed temporal techno-economic analysis and optimisation of off-grid green ammonia systems within these hubs.

The study shows that due to the high-quality co-located wind and solar resources, parts of Australia have a high potential for cost-competitive ammonia production, particularly when flexibility in the HB and associated industrial processes is assumed. We estimate that production costs in 2030 of AU$659 to AU$768/tonne could be achieved in Tennant Creek and Pilbara, respectively. These production sites could produce cost-competitive ammonia if gas prices remain high (above AU$14/MBtu) or carbon prices exceed AU$123/tonne concurrent with gas prices below AU$6/MBtu.

The role of flexibility in the HB process is likely to be contentious. Typically, large industrial processes are run at high capacity factors, often only shutting down for periodic maintenance, perhaps only every few years. Building and operating a plant that can be flexible needs to be preceded by re-designing for efficiency and avoiding rapid degradation of equipment from thermal stress.

This study has also identified complimentary seasonal variability in the supply and demand of renewable ammonia in Australia and various locations in the Northern Hemisphere. Implementing this would require the shipping fleet logistics to be responsive to seasonal demand. Further study is required to establish if this would be cost effective, and whether there is any possibility of dual use of assets by shipping other commodities at other times of the year.

Future work will compare off-grid ammonia production with grid-connected ammonia in terms of embedded emissions, economic viability, and operational strategies. The impact of the temporal output and delivery commitment on optimal system design is less discussed in the literature, which is worth considering in model development. Comparing ammonia production between different technologies, such as AE, PEM, and high-temperature solid oxide electrolyzer cell (SOEC) is also worthwhile exploring. Another area for further research is hydrogen carrier comparisons in terms of conversion efficiency and their associated shipping costs.

The success of global production, transport and trade of renewable energy carriers such as ammonia will require further careful analysis as the interactions between various parts of the system are complex. To support this work, governments acting as suppliers and or consumers of ammonia will need to form close alliances with each other and the ammonia industry to attract large-scale institutional investments.

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