

The New Steel Map: Reconfiguring Supply Chains Around Renewable Resources

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Abstract

Steel is an indispensable component of our physical environment and the most consumed metal on earth at 2 billion tonnes per annum. Continuance of this consumption and production pattern is incongruent with climate change mitigation; steel production is deeply dependent on fossil fuels with the sector emitting about one-tenth of energy-related global greenhouse gas emissions. Decarbonisation must commence immediately to reach near zero-emissions by 2050 and not exceed the allocated 30-year carbon budget aligned to a 1.5°C global warming trajectory. This presents a hefty challenge given the fundamental change in energy inputs required, consequent modification of metallurgical processes, and restructuring of the supporting supply chains. Yet, a significant opportunity lies in transitioning the industrial sector towards electrification with zero-carbon electricity inputs. In terms of physical pathways to near zero-emissions, the current literature body focuses on process level improvements, whilst supply chain assessments from raw materials to markets are largely absent. The energy paradigm shift introduces multiple novel supply chain elements worth exploring, including green hydrogen and iron trade, matching variable renewables with processes of varying flexibility, and opening of green markets under carbon policies. This literature gap is addressed in this thesis through mathematical modelling and geospatial analysis at multiple scales, spanning individual processes to the complete supply chain, and applied in local, regional, and global contexts.

The systems-based, locational research agenda allows exploration and evaluation of novel configurations for renewables-based steel supply chains. The technological focus is on hydrogen-based direct reduction of iron followed by the electric arc furnace, which reduces emissions to near zero and is rapidly reaching commerciality. The most significant tangible contributions of this thesis are the facility-level and supply chain optimisation models, which can be applied in any locality or region of interest. However, only through the meaningful case study analyses did critical insights emerge, of particular interest: (i) it is economically and energetically rational to reconfigure steel supply chains around high-quality renewables and iron ore deposits; (ii) co-locating hydrogen and iron production, and dislocating iron and steel production through green iron trade, introduces a valuable trade paradigm that takes advantage of upstream renewables whilst maintaining downstream market strongholds, (iii) iron ore producers have an integral part to play in the green steel transition, and a significant opportunity exists for these nations to transition from predominantly extractive to manufacturing economies, (iv) regional trade alliances and carbon policies are critical to green steel transitions, and (v) sectorial decoupling from fossil fuels requires well-timed investments and low-carbon energy system integration. Resource reallocation in the steel industry calls for supply chain restructuring; carrying over of fossil-based legacies will be a lost opportunity.

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Journal articles

- Devlin, A., Kossen, J., Goldie-Jones, H., & Yang, A. (2023). Global green hydrogen-based steel opportunities surrounding high quality renewable energy and iron ore deposits. *Nature Communications*, 14(1), 2578. <https://doi.org/10.1038/s41467-023-38123-2>
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This thesis is dedicated to future generations – may your world not be destructed by climate change, nor conflict. This research has shocked me at times, in the revelation of just how significant the challenge is to decouple fossil fuels from industry; equally, understanding the progress to-date and breakthrough technologies in the pipeline has reinforced my belief in humankind's capacity to do so.

List of Acronyms

BF	Blast furnace
BOF	Basic oxygen furnace
BOG	Boil-off gas
CAPEX	Capital expenditures
CBAM	Carbon border adjustment mechanism
CCU	Carbon capture and utilisation
CCUS	Carbon capture, utilisation and/or storage
CCS	Carbon capture and storage
CF	Capacity factor
CFR	Combined cost and freight
CGH ₂	Compressed gaseous hydrogen
CoV	Coefficient of variation
CO _{2e}	Carbon dioxide equivalents
DR	Direct reduction
DRI	Direct reduction of iron / direct reduced iron
EAF	Electric arc furnace
EOL	End of life
ETS	Emissions trading scheme
FC	Fuel cell
FOB	Free on board
FTE	Full time equivalent
GAMS	General Algebraic Modelling System
GHG	Greenhouse gas
GVA	Gross value added
H ₂ -DRI	Hydrogen-based direct reduction of iron
HBI	Hot briquetted iron
I-O	Input-output
LCOA	Levelised cost of ammonia
LCOE	Levelised cost of electricity
LCOH	Levelised cost of hydrogen
LCOS	Levelised cost of steel
LH ₂	Liquefied hydrogen
LHV	Lower heating value
LS	Liquid steel
ML	Machine learning
MOE	Molten oxide electrolysis
NG	Natural gas
NPV	Net present value
OHF	Open hearth furnace
OPEX	Operational expenditures
OSBF	Open slag bath furnace
PEMFC	Polymer electrolyte membrane fuel cell
RE	Renewable energy
SAF	Submerged arc furnace
SOFC	Solid oxide fuel cell
SFS	Semi-finished steel
SMR	Steam methane reformation
VRE	Variable renewable energy

Currencies

AUD	Australian dollar
UAH	Ukraine hryvnia
USD	United States dollar

Nations and regions

AU	Australia
BR	Brazil
CA	Canada
CL	Chile
CN	China
EU	European Union
GN	Guinea
IN	India
IR	Iran
JP	Japan
KZ	Kazakhstan
MX	Mexico
PE	Peru
RU	Russia
SE	Sweden
TR	Turkey
UA	Ukraine
US	United States
ZA	South Africa

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Chapter 1. Introduction

1.1 Background and motivation

Steel is a critical material in the construction, automotive, aviation, and defence industries, and essential in the clean energy transition to produce wind turbines, electric vehicles, and zero-emissions buildings. Steel production, however, is energy-intensive and consequently emissions intensive due to the deep dependence on fossil fuels. The sector consumes 20% of global industrial energy use (845 million tonnes of oil equivalent (Mtoe)), with coal supplying 74% of energy inputs for thermal and electrical energy as well as chemical energy for iron ore reduction (IEA, 2020b). Sectorial emissions amounted to an extensive 3.8 billion tonnes of carbon dioxide equivalents (Gt CO₂e) in 2021, equivalent to 10.5% of global energy-related CO₂ emissions (which totalled 36.3 Gt CO₂ (IEA, 2021a)). The sector's greenhouse gas (GHG) emissions are predominantly CO₂ with a minority of methane from metallurgical coal mining and natural gas extraction and refinement. Proportionally, about 65% of emissions are attributed to on-site industrial processes (scope 1), 15% to offsite electricity combustion (scope 2), and 20% offsite material manufacture (upstream scope 3) (IEA, 2021c; MPP, 2022; SBTi, 2023). Global commitment to climate change mitigation was ratified under the 2015 Paris Agreement by 195 countries representing over 98% of global GHG emissions and 98% of global steel production (Iran excluded) (United Nations, 2023). For a 55% likelihood of limiting global warming to 1.5°C, the steel sector has a carbon budget (covering scope 1 and 2) of 56 Gt CO₂ across the three decades from 2020 to 2050 (MPP, 2022) and for a 67% likelihood the budget is further constrained to 37 Gt CO₂ (Teske et al., 2022). The emissions intensity of steel must reduce from the current global average of 1.9 tonnes of CO₂ per tonne of steel (t CO₂/t steel) (worldsteel, 2020b) to near zero, whilst meeting the forecasted increase in global demand from 1.95 billion tonnes per annum (Btpa) (worldsteel, 2022), to 2.5 Btpa by 2050 if material sufficiency and efficiency measures (e.g., lightweighting, increased durability, improved circularity) are not realised (Bataille et al., 2021; MPP, 2022). Steel has an indispensable role in society, but the manufacturing processes and supply chains that support them, from raw materials to markets, require deep transformation.

The steel sector's current production landscape is geographically diverse, but technologically homogenous. Present steelmaking processes can be classified into three main technology routes: blast furnace followed by basic oxygen furnace (BF-BOF), scrap-charged electric arc furnace (scrap-EAF) and direct reduction iron followed by electric arc furnace (DRI-EAF). Globally, the BF-BOF route produces 71% of steel (1385 Mt), with 23% via the scrap-EAF route (447 Mt) and 6% via the DRI-EAF route (119 Mt) (Midrex, 2022; worldsteel, 2022). BF-BOF production is the most pollutive, relying on coal for energy and iron ore reduction, emitting an average of 2.4 t CO₂/t steel globally, whilst the DRI-EAF route mostly uses natural gas as the feed gas and produces on average 1.2 t CO₂/t steel, and the scrap-EAF route eliminates the need for ore reduction altogether, emitting 0.5 t CO₂/t steel (all considering scope 1 and 2 emissions) (MPP, 2022). Fifty countries account for 99% of global steel production, but just three countries account for 66% with a distinct concentration in Asia: China

dominates market share (54%), followed by Japan (7%) and India (5%) (worldsteel, 2022). There is significant variation in national steel emission intensities which reflects the quality of input materials, quantity of scrap charging, electricity sources, and process energy efficiency, among others; in t CO₂/t steel (scope 1 and 2), BF-BOF emissions range from 1.75 (Canada) to 2.75 (India and Poland), and EAF from 0.3 (France) to 1.6 (India) (Hasanbeigi & Springer, 2019). Sectorial achievement of near zero-emissions steel by 2050 requires collective global effort.

Electrified steelmaking processes can be readily decarbonised with the sourcing of renewable power, but for ironmaking processes which need both thermal and chemical energy inputs, the solution is not as simple. Steel production can be categorised into two major production categories: (i) ore-based (termed primary production), where iron ore must first be chemically reduced into metallic iron, then further impurities removed and alloys added, and (ii) scrap-based (termed secondary production), where recycled scrap steel is melted, impurities removed, and alloys added. Although in practice, this binary distinction is rare; scrap is often added to primary production, and fresh metallic iron to secondary. Whilst a scrap content (as a portion of total Fe charge) of 10-15% is typical for integrated BF-BOF production (with a technical limit of 25%; Kildahl et al. (2023)), the scrap content varies widely in EAF production, up to 100%. The emissions and energy intensity of scrap-based production is significantly less than that of ore-based production, therefore technology substitution seems obvious. However, constrained scrap availability and persisting contaminants, like tin and copper, limit expansion (Daehn et al., 2017), such that the scrap-based portion of global steel production in 2050 has been estimated at about 50% (Stefan Pauliuk et al., 2013). This represents about double the current secondary steel market share, but the remaining 50% of demand must be met by primary production. In addition, since scrap availability is determined by the age of steel stocks, the critical resource is concentrated in developed nations where large quantities of steel contained in buildings, infrastructure, vehicles, and machinery are reaching the end of their lifetime (Wang et al., 2021). The regionally unequitable resource constraint on decarbonisation potential has prompted the leading sectorial global multi-stakeholder standard (ResponsibleSteel, 2021) and science-based emissions reduction pathway guidance (SBTi, 2023) to develop GHG emission thresholds as a function of scrap, with 'near zero' classified as 50-400 kg CO_{2e}/t steel in the former (covering scope 1, 2 and upstream scope 3 emissions). Moreover, the greatest challenge for sectorial decarbonisation is ore-based production, which is currently dominated by blast furnaces. Substantially altering or replacing BF's is no easy feat; they carry strong asset inertia due to long campaign lives (the global historical median is 17 years (Vogl et al., 2021b), and are in excess capacity (the global estimate in 2022 was 26% (OECD Steel Committee, 2023)). The decarbonisation of both primary and secondary steel production must occur simultaneously; increasing the scrap portion in one manufacturing plant will simply displace it from another and have no effect on global sectorial emission reductions.

The shift from the Iron Age to the Steel Age occurred in 1856 when Henry Bessemer successfully demonstrated the conversion process, driving the second industrial evolution (Gale, 1973). For nearly 170 years, primary steel supply chains have been configured to minimise costs by strategically locating plants within proximity, or with efficient transport routes, to both upstream metallurgical coal/iron ore

mineral resources, bulk transnational freight is frequently relied on; the largest shipping vessel in the world is the Valemax (named after the iron ore mining company) of 400,000 dwt which specifically transports iron ore from Brazil to China. Australia and China stand out as global quarries for the steel sector: 34% of iron ore is produced in Australia (912 Mt in 2021), followed by Brazil (16%), China (15%) and India (10%) (U.S. Geological Survey, 2022), whilst 58% of operating metallurgical coal mines are located in China, 16% in Australia, and 12% in Russia (GEM, 2023b). A global trend of diminishing iron ore reserve quality (due to selective extraction) has caused increased reliance on beneficiation processes to remove gangue material (i.e., impurities). The global iron ore inventory is estimated at 180 Bt crude ore, containing 85 Bt elemental iron (Fe) which indicates an average Fe content of just 47%, far lower than BF-grade (65%-Fe) or DR-grade (67%-Fe) requirements. The immediate product from steelmaking, crude steel, is not in a tradeable form, it must be cast into a semi-finished state (blooms, billets, or slabs) or further processed into a finished product for transportation. Flats (e.g., coils, sheets, plates, structural beams) and longs (e.g., rods, bars, sections) are the two main finished steel product categories. Due to plant-product specialisations, global steel trade is often necessary even if, by tonnage, a country could be self-sufficient. Nevertheless, the flow and transformation of materials and energy from source to final steel product is not locked-in – a fleeting yet immense opportunity arises to explore geographically divergent supply chains.

There are several low- and zero-emissions production processes in development, with some already commercialised, or on the cusp of industrial-scale deployment. Whilst incremental decarbonisation measures can lower sectorial emissions, including material sufficiency, material efficiency, energy efficiency, and biomass substitution, an industrial paradigm shift away from fossil fuels is required to reach near zero-emissions. Direct reduction using green hydrogen, direct electrification, and carbon capture, utilisation, and storage (CCUS) are the three deep decarbonisation measures the sector will likely depend on. Each innovation area pertains technologies of varying emission reduction capacities, technological maturities, economic feasibilities, and relative strengths and limitations (Fan & Friedmann, 2021; Fishedick et al., 2014), as detailed in Section 2.1. In brief, although CCUS is considered a technically viable solution that can be retrofitted to existing BF-BOF facilities (as well as DRI-EAF facilities), the large number of emission points makes it costly and inefficient to capture CO₂. Comparatively, production by green hydrogen-based direct reduction of iron followed by the electric arc furnace (H₂-DRI-EAF) can eliminate 98% of conventional integrated steelmaking emissions and is due to reach commercialisation by 2026-27. Other 'breakthrough' technology such as direct iron electrolysis is being developed, yet the technology has not yet reached pilot-stage so eventual commercialisation may be too late to gain significant market share. Considering the imminent need to decarbonise and the current landscape of steel decarbonisation technology, this thesis focusses on optimising green H₂-DRI-EAF production, its renewables-based supply chains including international trade routes, on the pathway to near zero-emissions by 2050.

The H₂-based direct reduction route unlocks new supply chain opportunities. In comparison to integrated BF-BOF steel production where ironmaking and steelmaking processes cannot be separated

due to the molten state of the iron product from BF operations, the DRI-EAF route can be completely dislocated due to the solid sponge iron product from DRI operations. The tradeable intermediary product, hot briquetted iron (HBI), can be stored and shipped overseas with relative ease (although some concerns remain around oxidation (Daghagheleh et al., 2023)), meaning, for example, that DRI plants could be located nearby iron ore deposits and EAF plants nearby customers. In addition, the hydrogen economy presents opportunities to utilise energy carriers for storage and transport, and to optimise flexible production systems using variable renewable energy (VRE) sources – critical, given it is far less efficient to transport H₂ in comparison to thermal coal. Source-to-user energy efficiency is critical for all energy applications, but especially for energy-intensive industrial sectors. Moreover, the shift from coal-based to renewables-based production is calling for novel supply chain configurations.

1.2 Objectives

The overarching research aim is to support steel sector decarbonisation by generating critical insights into, and develop templates for, the establishment of technically feasible, economically attractive, and resource-efficient renewables-based steel supply chains. By framing industrial relocation as an enabler for industrial decarbonisation, one can redefine the movement of energy and materials from source to crude steel, and then onto demand markets. Through a systems engineering lens and a geospatial explicit approach, the research is poised to develop effective supply chain solutions for iron ore-dependent (i.e., primary) steel production at local, regional, and global level. The horizon for analysis is set to the year 2050 when, globally, about 2.5 Btpa of near zero-emissions steel may be needed.

The following research objectives are defined:

Objective 1. Investigate the emerging energetics and techno-economics of green H₂-based steelmaking, over time and space. Define the critical factors underpinning cost-competitive production and appraise localised energy-production systems for their ability to pair intermittent renewable energy with production processes of ranging flexibility.

Objective 2. Explore the energy- and cost-saving benefits of novel trade paradigms across the green H₂-based steel supply chain, notably the utility of H₂ and HBI transport.

Objective 3. Evaluate desirable green steel project investment timings, especially considering the physical inertia of existing assets, and transitional energy sources and technologies.

Objective 4. Assess supply chain opportunities and obstacles within the given local or regional context, in terms of natural resource availability and quality (e.g., iron ore, scrap, and land), as well as financial and geopolitical constraints.

Objective 5. Deliver relevant and practical insights to industry practitioners and policymakers.

1.3 Thesis structure and technical scope

	Analytical focus	Spatial and temporal scale	Production scale	Computational analysis (inc. spatial + temporal resolution)
Chapter 3 	Facility-level optimisation of green H ₂ -DRI-EAF steel production using islanded solar and wind energy and local iron ore resources.	Global (>300 iron ore deposits) Years for model projection: 2030, 2040, 2050	1 Mtpa	Green H ₂ -DRI-EAF steel production optimisation model evaluated energy and mass flows for each 8760 hours of a year, executed for 44 regions within 17 important iron ore producing regions, and repeated using 5 historical years of solar and wind energy data. Machine learning applications expanded analysis to over 300 iron ore deposits.
Chapter 4 	Analysis of favourable green H ₂ -DRI-EAF steel supply chains to optimise natural resource availability.	Transnational (Australia-Japan strategic partnership) Years for model projection: 2030, 2050	40 Mtpa (equivalent to Japan's steel demand in 2050, and Australia's current iron ore exports to Japan given ~1.5t ore/t steel)	Evaluation of 12 unique cases using a steel production and trade simulation model, varying in supply chain configuration, H ₂ energy carrier (LH ₂ , NH ₃) and year (2030, 2050). Compared on the basis that all energy had to be generated in the Pilbara region of Western Australia.
Chapter 5 	Steel production and trade optimisation in the transition from the current fossil-based to future renewables-based steel sector.	National production within regional trade network (Ukraine, EU) Years for model projection: 2030, 2040, 2050	Up to 22.5 Mtpa (determined by dynamic MFA for each modelled year)	Green steel transition optimisation model which evaluated energy and mass flows in a single year, executed for two distinct scenarios based on war outcomes (Slow Recovery or Strong Recovery).

Figure 1.1 Methodological overview of the three original research chapters, including scope, scale, and resolution.

The thesis comprises a literature review followed by three original research chapters which each contain an introduction, methods, results, discussion, and conclusion. The objectives of this thesis are tackled in hierarchical order (i.e., Objectives 1, 2 and 3 align with Chapters 3, 4, and 5, respectively), with objectives 4 and 5 being addressed in all chapters. The thesis has been structured to build in supply chain complexity, starting with the simplest configuration for green H₂-based steel production in which electrolysis, iron ore reduction and steelmaking are all co-located close to the iron ore deposit, and expanding to multiple configurations with diverse export markets, as detailed in Figure 1.1.

The integrated thesis format has been adopted, where published or under-review papers make up the original research chapters. Slight adjustments have been made to align formatting and terminology and all currencies converted to United States dollars (USD) - Chapter 4 was originally in Australian dollars (AUD), for which an exchange rate of 0.65 USD/AUD applied. To minimise repetition of information, general framing of the industrial decarbonisation challenge and review of previous studies to identify literature gaps have been removed from each chapter's introduction, and instead synthesised in Chapter 1 and Chapter 2. Hence, chapters roughly match the publication length, and further details on the methods and results are presented in the respective Appendices.

The thesis is organised as follows:

Chapter 1 provides background information, the study's motivations, and a structural overview.

Chapter 2 reviews the current literature on decarbonised steel production technologies and systems engineering approaches to steel decarbonisation, including energy systems modelling and supply chain

assessments. Gaps are then highlighted and the pathway for this thesis to contribute to the overall literature body devised.

Chapter 3 optimises green H₂-DRI-EAF steel production at facility-level, initially in 44 regions of the top 17 important iron ore producing regions, with global expansion to over 300 iron ore deposits through applied machine learning (ML) techniques. Both islanded renewable energy systems (using solar and wind), and grid-based energy systems are compared in terms of process flexibility, production costs, and emissions. This locational scoping study captures the geographical landscape of projected green steel market competitiveness and provides insights into the changing market dynamics given the new accounting compared to fossil-based steel production.

Chapter 4 investigates novel binational supply chain configurations for the green H₂-DRI-EAF steel production route to evaluate the utility of H₂ and HBI trade as well as the changing dynamics within traditional supplier-producer networks. The Australia-Japan trade partnership was chosen for analysis due to the distinct allocation of resources: Australia (AU) is the world's largest iron ore producer, has a large land mass, and significant solar and wind energy potential, whilst in comparison Japan (JP) is the world's second largest steel producer, but with minimal available land and renewable energy capacity, and an aging population and therefore diminishing workforce. Importantly, Australia and Japan have already demonstrated collaboration across H₂ and steel value chains. Industrial relocation is presented as a mutual opportunity to take advantage of Australia's plentiful resources, whilst maintaining Japan's steel output and market competitiveness.

Chapter 5 investigates green steel transition strategies for nations with legacy coal-based steel production assets, on the pathway to near zero-emissions by 2050. The supply chain optimisation study clarifies what technology should be invested in (type and capacity), when (2030, 2040 or 2050), and where (of 73 locations comprising 1°x1° grid spatial resolution which is about 111 km (latitude) x 73 km (longitude)). A range of technology options (including the DRI-melter-BOF route for lower grade ores) and energy inputs (including natural gas and nuclear power) are considered. The transitions framework incorporates techno-economic, policy and geopolitical factors. A projected post-war Ukraine (UA) is chosen as the case study due its global interest, the opportunity presented by prospective European Union (EU) accession (and consequent imposed carbon policies) and anticipated international funds that will become available for the country's reconstruction.

Chapter 6 summarises the key findings and contributions of the body of work and consequent implications for stakeholders within the steel decarbonisation community. Research limitations are also discussed and future research directions identified.

Across the three research chapters (Chapters 3-5), the supply chain scope expands from co-located H₂-DRI-EAF production, then to three different binational supply chain configurations, and finally a plethora of different supply chain configurations under a sectorial optimisation framework. The number of energy and mass flows increased dramatically, which could be managed by more sophisticated modelling methods and a reduction in spatial coverage: from global, to transnational, then national with

regional trade links. Hence, a trade-off was managed between supply chain complexity and spatial scope, whilst maintaining high spatial granularity.

For consistency, the production boundary applied throughout the body of work was up to the point of crude steel where solidification first occurs, as shown in Figure 1.2. The continuous casting route which produces semi-finished steel (slab, billet or bloom) was chosen as it is a comparable point for nearly all steel products, and accountable for about 85% of energy consumption for hot rolled steel produced via the DRI-EAF route (for scrap-based production, this portion is much lower due to absence of iron ore reduction) (Price et al., 2001).

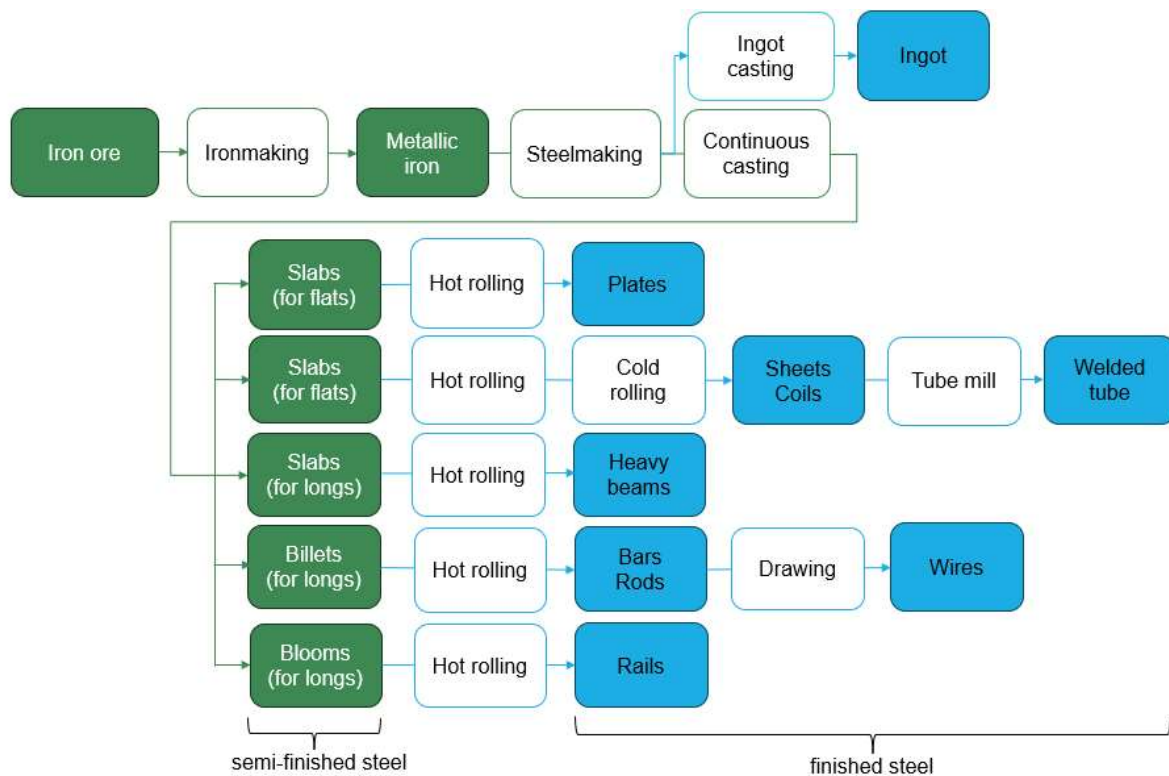


Figure 1.2 Simplified diagram of steelmaking operations showing processes and products from iron ore to finished steel products, with colour delineation indicating the production boundary (energy inputs not shown). Green colouring indicates processes within the assessed production boundary (up to semi-finished steel, continuous casting being the final process), whilst blue colouring indicates processes external to the boundary.

Also throughout, the primary economic measure used to compare technologies, supply chains, and/or locations was the levelised cost of steel (LCOS) which is a calculation of the net present value (NPV) of the total project costs over its lifetime, over the NPV of all steel produced over its lifetime (assumed consistently to be 20 years). This was often complemented by the levelised cost of electricity (LCOE), levelised cost of hydrogen (LCOH) and levelised cost of ammonia (LCOA) as core constituents of the fossil-free production system.

Chapter 2. Literature Review

Overview

This chapter explores previous work related to the topic of steel sectorial decarbonisation and identifies literature gaps that need to be tackled to optimise, commercialise, and scale-up solutions. First, near zero-emissions steel production technology options are assessed in terms of their technical viability and economic feasibility, and related project developments discussed. Second, systems engineering approaches to steel decarbonisation are explored, related energy system modelling and supply chains assessments discussed, and key research gaps listed.

Sections 2.1 and 2.3 of this chapter include work published within the following report; however, substantial modifications have been made to broaden the original UK context to the global steel sector: Devlin, A., & Markkanen, S. (2023). *Steel sector deep dive: How could demand drive low carbon innovation in the steel industry*. Cambridge Institute for Sustainability Leadership (CISL). https://www.cisl.cam.ac.uk/files/sectoral_case_study_steel.pdf.

Among all authors who contributed to the published report, A.D. analysed and categorised the literature, conceptualised the content, and wrote the manuscript. S.M. supported the literature analysis, provided useful feedback in the conceptual stage, and revised the manuscript.

2.1 Decarbonised steel production routes

To eliminate emissions from the global steel sector, the deeply engrained dependency on fossil fuels must be dramatically amended. Both supply-side (i.e., steel producers) and demand-side (i.e., construction, automotive, machinery and product sectors) are responsible for leading this change. A range of incremental measures exist which are important in the short-term; however, attention is drawn to the deep decarbonisation innovation areas of hydrogen (indirect electrification), direct electrification, and carbon capture and storage, which will be relied on to proactively mitigate, or retrospectively capture, emissions from iron and steel production (refer to Figure 2.1).

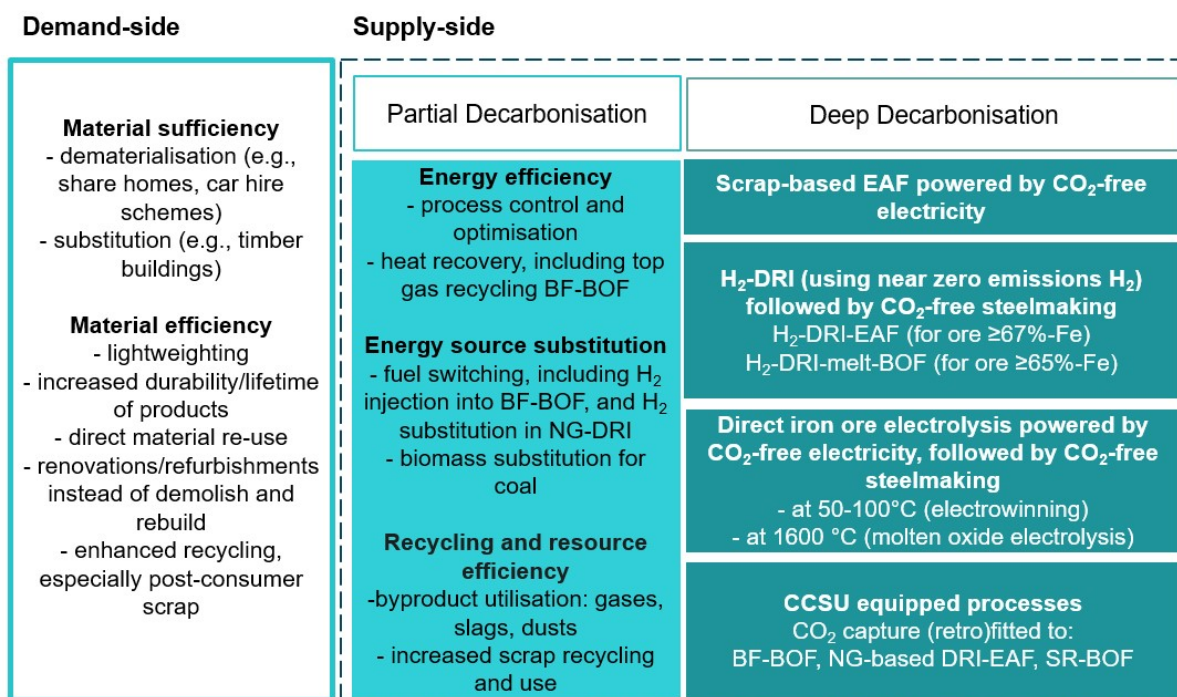


Figure 2.1 Emission mitigation opportunities for the steel sector. Measures encompass demand-side material sufficiency (reducing absolute steel demand) and efficiency (reducing the steel required to perform the same function), as well as a range of supply-side technology interventions for partial and deep decarbonisation.

It must be clarified that there is no universal definition for ‘green steel’, nor standard emissions boundary or GHG accounting method, which unfavourably causes incomparability across steel products and plants, confusion for industry stakeholders and instances of greenwashing (Hasanbeigi, 2023). Whilst one organisation has introduced a product-based green steel threshold which is agnostic to scrap charge (Global Steel Climate Council, 2023), the majority of the sector has reached consensus that the threshold should be a function of scrap (refer to Figure 2.2), effectively distinguishing between the ease of decarbonising scrap-based production and comparative difficulty of decarbonising ore-based production, as well as the inequality of scrap distribution. In this work, green steel has been defined as steel produced in the (near full) absence of fossil fuels, used interchangeably with ‘near zero-emissions steel’ and ‘fossil-free steel’. This definition is extended to ‘green HBI’, the intermediary product between DRI and steelmaking. The minor emissions allowance is due to the fact that steel is an alloy of iron and carbon. If fossil fuels are completely removed from the process as ore reductants and thermal energy inputs a minor amount of carbon must be added during steelmaking, producing a small amount of CO₂ alongside the CO₂ produced from the graphite electrodes in electric smelting operations, totalling less than 3% of BF-BOF emissions (Vogl et al., 2018)

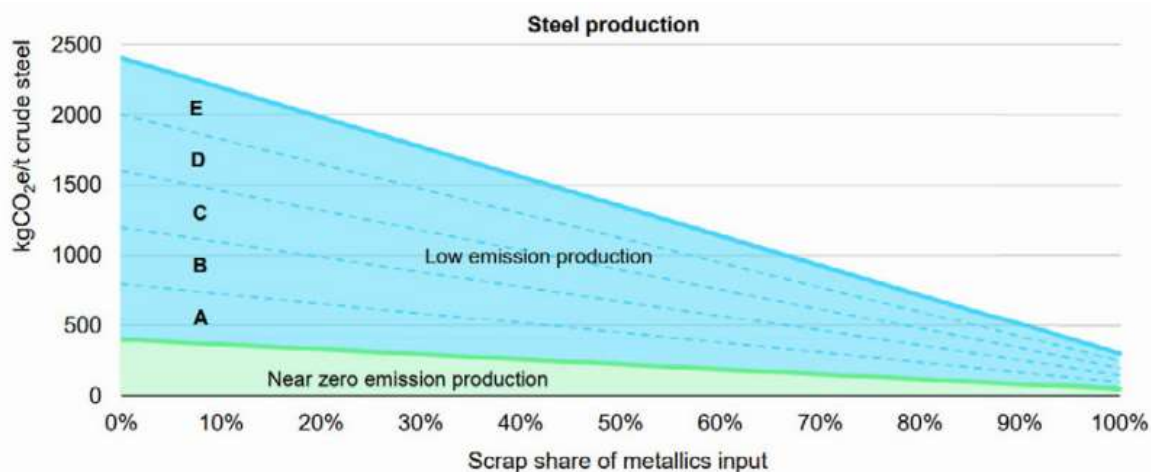


Figure 2.2 Low and near zero-emission crude steel production thresholds as a function of scrap use. Published by IEA (Levi et al., 2022) which aligns closely to that presented in ResponsibleSteel's International Standard v2.0, Principle 10.6 (ResponsibleSteel, 2022). The near zero-emissions production threshold is equal to 400 kg CO₂e/t crude steel for 100% ore-based production, and 50 kg CO₂e/t crude steel for 100% scrap-based production, inclusive of scope 1, 2 and upstream scope 3 emissions.

The most promising solutions for significant sectoral emission reductions are discussed in this first section of the literature review, with an intentional focus on ore-based production.

2.1.1 Improved material circularity and contaminant removal will increase the share of scrap-based EAF production

Scrap-based steelmaking powered by renewable electricity offers the simplest, and most energy- and cost-efficient route to green steel production. Yet, the growth of this closed-loop recycling production route is constrained by future scrap availability. In 2021, 29% of global steel production was via the electric route (worldsteel, 2022). This implies that around 620 Mt of scrap steel was utilised assuming that the electric route was dominated by scrap-based EAF production, and given a scrap consumption rate of 1.1 t scrap/t steel considering remelting yield losses (Birat, 2020). Scrap production and consumption was also largely localised with just 18% of steel scrap (110 Mt) traded globally (worldsteel, 2022). Secondary material flows depend on end-of-life steel stocks and recycling rates, the former which is subject to severe regional inequalities. By 2050, developed nations such as the European Union (EU) and North America could completely meet steel demand with available regional scrap, whilst China could meet 50% of demand, yet developing nations including India and some African states may only be able to meet 5% (Watari et al., 2023). Scrap flows are constrained, and both spatially and temporally variable, limiting scrap-based EAF production expansion.

Whilst scrap steel is theoretically infinitely recyclable without loss of properties, technical, economical, and logistical challenges have constrained the global scrap recycling rate to around 85% (Tata Steel, 2023). By sector, global steel recovery rates are estimated at 85% for construction, 90% for automotive, 90% for machinery, and 50% for electrical and domestic appliances (worldsteel, 2023). There are three main scrap types: home scrap (excess materials from within steel plants themselves), industrial/prompt scrap (from downstream manufacturers) and end-of-life (EOL) scrap (from post-consumer products). Prompt scrap is especially abundant in automotive manufacturing - just 55% of the steel purchased by

car manufacturers ends up in the vehicle (Allwood et al., 2019). Pre-consumer scrap recycling rates are 99-100%; obsolete scrap recycling is where inefficiencies occur due to inadequate recycling systems, persistent contaminants, and diminishing economics for lower quality scrap. Scrap contains many contaminants, most of which can be removed via oxidation and slag formation, however, tramp elements (e.g., copper and tin) are very difficult to remove and impair metallurgical processing (Nakajima et al., 2011). EOL scrap from construction, especially structural steel, is incredibly valuable due to the low contaminant levels, whereas tramp elements are prevalent in automobiles, appliances, and machinery so dilution practices must be utilised (Daehn et al., 2017). Improvements to EOL scrap recycling systems and contaminant removal processes would dramatically increase iron-containing material retention and enhance scrap-based steelmaking potential. A misconception exists within the industry that scrap-based steelmaking cannot produce high-grade steels; so long as scrap sorting, recycling and quality control processes are proficient, specialty steels can be produced without any metallic iron inputs. As a testimony to this, Liberty's EAF facility in Rotherham is a specialist manufacturer of high-end alloys and stainless steels, serving the aerospace and defence sectors and specialist engineering applications (Liberty Specialty Steels, 2020). Contaminant control in scrap recycling is essential to expand typical EAF product lines.

2.1.2 Biochar can substitute coal, but is an unfeasible solution at scale

There is potential for emissions reduction in steelmaking through biomass integration, yet constrained resource availability and broader sustainability concerns limit growth. Biomass, including agricultural residues (straw, corn stalks, sugarcane bagasse), wood and forest residues (sawdust, bark, timber harvesting, logging residues) and industrial waste, can be pyrolysed or gasified to produce biochar, a renewable, carbon-rich feedstock suitable for coal substitution (Amalina et al., 2022; Mousa et al., 2016). Partial substitution of coke is also possible for biochar with a fixed carbon content greater than 80% and calorific value greater than 27 megajoules per kilogram (MJ/kg). The greatest potential for biochar use in BF operations is to substitute pulverised coal injection (PCI), with a maximum injection rate of 220 kg/t hot metal and emissions reduction up to 25% (Safarian, 2023). Critically, biomass resources and land availability for biomass cultivation are finite, and the steel industry is not a priority downstream user. Biomass production must firstly be allocated to food production, and then industries which can't be electrified, for example, aviation and marine shipping. Favourably, biochar can also be used in EAF steelmaking to replace fossil-based carbon additives that carburise the melt (recall that steel is an alloy of iron and 0.2-1.5% carbon), and the low volumes required mean that biomass availability is not a barrier to adoption. Moreover, the viability of biomass utilisation is undermined by the inherent sustainability risks from monoculture landscapes including the loss of biodiversity, nutrients, and carbon sinks (Wichtmann & Wichmann, 2011). Partial biochar substitution in the short-term may be feasible, but overall contribution to sectorial emissions reduction will likely be marginal.

2.1.3. Emissions abatement from CO₂ capture is highly constrained, and BF-BOF retrofit remains untested

CO₂ capture in an integrated BF-BOF plant is subject to challenges derived from the magnitude of emission points and the relatively low CO₂ concentration of each point source. Besides, CCUS using

process gases does not generally result in near zero emissions and “negative emissions” are only achievable (even in principle) by using non-fossil carbon. Emissions are released from the BF and the BOF, as well as multiple auxiliary units: coke oven, sinter plant, hot stoves, lime kiln, and power plant. From a techno-economic perspective, capturing CO₂ from just the BF gases (25%vol CO₂) or the power plant flue gases (30%vol CO₂) are the most effective means of emissions abatement as the sources with highest CO₂ concentration, but plant-level emissions reduction for each intervention is limited to about 40%. Simultaneous CO₂ capture from BF, hot stoves and power plant gases can reduce total plant emissions by 80%, however, costs and energy consumption for solvent regeneration also increase (Normann et al., 2019; Sundqvist et al., 2018). For post-combustion capture at steel plants using amine scrubbing, the average cost estimate from literature is \$65/t CO₂ with a maximum of \$120/t CO₂ (Leeson et al., 2017). Increased process efficiency could be attained by utilising excess heat for steam production to drive the capture and regeneration processes (Biermann et al., 2019), incorporating top gas recycling (Fischedick, et al., 2014), and/or integrating calcium-looping lime production (Tian et al., 2018). Biomass energy and CCUS could be utilised simultaneously, with estimated costs of \$85/t CO₂ avoided for an average EU steelmaker (Mandova, et al., 2019). The prospect of net negative lifecycle CO₂ emissions are only possible in cases of intensive CO₂ sequestration during the biomass growth phase, extensive site-wide CO₂ capture, and permanent underground storage of CO₂ (Tanzer et al., 2020). Retrofitting the existing global BF fleet with CO₂ capture technology is where most research has been focussed; however, direct reduction and smelting reduction (SR) furnaces (which utilise non-coking coal and a range of ore products - lump, pellets and/or sinter (Gojiæ & Koþuh, 2006)) are also probable candidates. Ultimately, the viability of CCUS systems depends on point capture efficiency and the absolute emissions abatement at plant-level.

Following capture, CO₂ is stored or utilised, and the permanency of this second step is a fundamental requirement for emissions abatement. For storage in geological reservoirs such as depleted gas and oil fields and saline aquifers, CO₂ must firstly be compressed at the steel plant and then transported to the storage site where it is pumped underground to depths of more than 1 km (Blunt, 2010). CO₂ can also be mineralised and sequestered in solid form, but this solution is less mature. Uncertainty still exists around the feasibility of securing CO₂ in sedimentary pores for thousands of years due the complexity of the affecting subsurface physical and chemical processes (Kelemen et al., 2019). Alternatively, the captured CO₂ could be utilised, either directly, for example in enhanced oil recovery (EOR), carbonated drinks, and food preservation, or indirectly, to form hydrocarbons to produce chemicals, polymers, and fuels (Kamkeng et al., 2021). Use of captured CO₂ from integrated BF-BOF plants to produce synthetic methanol may be a profitable operation when optimised (Porter et al., 2022), and especially valuable as it can be recycled back into the steelmaking process as a fuel substitute for natural gas (Baena-Moreno et al., 2021). For every tonne of steel, about 3 tonnes of BF gas is produced, consisting of carbon monoxide (CO), carbon dioxide (CO₂), hydrogen (H₂) and nitrogen (N₂), and positively, advancements in gas separation techniques have enabled both pure CO and CO₂ streams to be acquired at steel plants, further enhancing utilisation potential (Ras, et al., 2019). Whilst carbon

capture and storage (CCS) is simply a waste mitigation technology, carbon capture and utilisation (CCU) offers byproduct valorisation and the prospect of negative emissions steel.

Commercial realisation of CCUS technology is eagerly awaited by industry, but project investments are scarce. A single commercial-scale CCUS installation exists in the global steel sector: Abu Dhabi's Al Reyada Project where CO₂ is captured from the NG-based DRI plant using amine absorption, then compressed and transported via pipeline to nearby oil wells for EOR (Abu Zahra, 2015), with capacity to inject up to 0.8 Mt CO₂ per year (Carbon Sequestration Leadership Forum, 2023). However, just 17% of the total plant emissions from the 3.2 Mtpa steel plant are estimated to be captured (Nicholas, 2023). The (retro)fitting of CO₂ capture technology to a BF-BOF plant has not yet been trialled, let alone commercialised (Fan & Friedmann, 2021). Although Tata Steel originally planned to build a full-scale smelting reduction plant with CCS in the Netherlands (following a successful pilot plant), this decision was overturned with a switch to DRI technology (S&P Global, 2021). Establishing and maintaining a system of capturing, storing and/or utilising the significant quantities of CO₂ produced from a steel plant presents logistical and financial difficulties which steel producers have not yet overcome.

2.1.4. Hydrogen-based direct reduction is maturing rapidly

Elimination of fossil fuels from iron production is achievable through the direct reduction route using 100% H₂ feed gas. As a modification of existing DRI operations (as depicted in Figure 2.3) which predominantly use natural gas (NG) as the reduction feed gas, the reduction byproduct would be pure water vapour (H₂O) instead of a mixture of H₂O and CO₂. If emissions-free hydrogen is procured, and auxiliary processes including the subsequent steelmaking step are renewably powered, near zero-emissions steel is produced. Today, H₂ is largely produced using steam methane reformation (SMR) which produces about 10 kg CO₂e/kg H₂, and if equipped with CCUS this would only decrease to 4 kg CO₂e/kg H₂ – a sizable amount of residual emissions due to CO₂ capture inefficiencies and methane emissions during natural gas production (Hermesmann & Müller, 2022). Utilising green H₂, whereby water is split into its constituent elements of H₂ and O₂ through renewable powered electrolysis, can reduce upstream emissions to zero. Multiple alternate low and zero-emission H₂ production methods exist, for example, extraction of naturally occurring H₂ in geological formations (gold H₂) (Zgonnik, 2020), methane pyrolysis (turquoise H₂) (Rahimi et al., 2019), or even electrified methane reforming (Wismann et al., 2019). Yet, green H₂ remains the solution with the highest emissions abatement potential and technology readiness level. Looking at announced projects, global electrolyser capacity could reach up to 365 GW by 2030 (IEA, 2023), which based on 75% electrolyser efficiency and 80% utilisation factor could produce 58 Mt H₂ per year and theoretically suffice nearly 1 Bt of green iron production (at 60 kg H₂/t steel; with 51 kg H₂/t steel being the theoretical minimum for DRI (Vogl et al., 2018)). H₂ may not only be used for DRI feed gas, but to supply thermal and electrical energy to the steel plant. Whilst substitution of NG with H₂ in DRI is a non-trivial process shift, it offers a streamlined strategy to near zero-emissions production.

Although a highly useful chemical, H₂ is very inefficient to store and transport due to its low volumetric energy density as a gas. For longer duration storage and longer distance transport, it must be

compressed (up to 700 bar for vehicles) and/or liquefied (at -253°C) or converted into a H_2 carrier. A high-potential carrier is green ammonia (NH_3) whereby N_2 is bound to H_2 through the Haber-Bosch process. Although NH_3 production requires additional energy, the roundtrip energy efficiency of storing and transporting liquefied NH_3 , including cracking the molecule back into H_2 when required for steelmaking, may still be greater than that of gaseous or liquefied H_2 (LH_2) due to its enhanced volumetric energy density and higher liquefaction temperature (at atmospheric pressure) of -33°C . Nevertheless, each storage and transportation method has unique challenges in production, storage, and utilisation (Salmon & Bañares-Alcántara, 2021; Wijayanta et al., 2019). Energy carriers like NH_3 and LH_2 will likely play an important role in green steel supply chains as both H_2 energy carrier and marine shipping fuel.

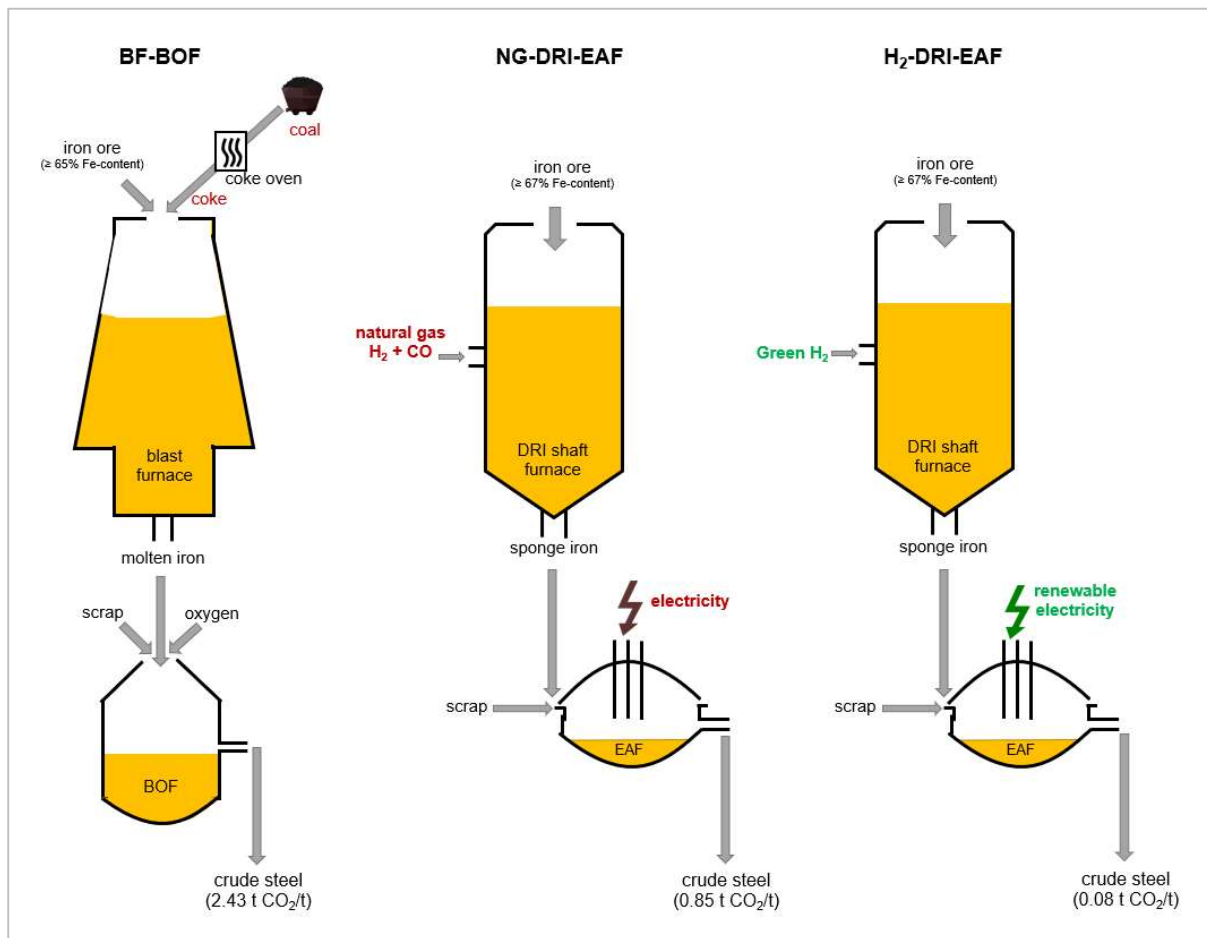


Figure 2.3 Current and emerging steel production processes with distinct material and energy inputs, technology, and emissions intensities. The emissions intensity (scope 1 and 2) for average BF-BOF production is $2.43 \text{ t CO}_2/\text{t steel}$, for NG-DRI-EAF is $0.85 \text{ t CO}_2/\text{t steel}$ and for H_2 -DRI-EAF is $0.08 \text{ t CO}_2/\text{t steel}$, for (MPP, 2022).

A key barrier to upscaling global H_2 -DRI capacity is iron ore quality. There are multiple DR furnace types, but the most common is the shaft furnace, a moving bed counter-current reactor, which operates at about 800°C where iron ore enters from the top and the reducing gas from the bottom (Parisi & Laborde, 2004). Operation below the melting point of iron produces a sponge iron product which offers

great utility as it can be briquetted into HBI or fed directly as hot DRI into the downstream steelmaking processes. Although, iron ore constraints are introduced: (i) high-quality iron ore is required as impurities are preserved, and (ii) iron ore must be in pellet form (with up to 30% lump) to provide enough mass to overcome the force of the gas and prevent sticking to the furnace (Linklater, 2021). If the gangue content is too high and the presence of contaminants including silica, alumina, and sulphur, are not controlled, the degree of metallisation will be limited, and downstream EAF processing will become very inefficient (Linklater, 2021). Simultaneously, the quality of global iron ore resources is decreasing due to selective extraction of high-grade ores which limits the expansion potential of H₂-DRI shaft furnace technology. There are some feasible solutions - research into H₂-DRI using fluidised bed technology has been explored (Wolfinger et al., 2022b) which utilises low grade ore fines (Zhang et al., 2023). Employing an additional smelting unit to remove impurities via slag production before subsequent steelmaking has also been proposed. This method may also take advantage of existing BOF assets for steelmaking as the product would be molten iron, forming the DRI-melter-BOF production route. Melter technology options include the submerged arc furnace (SAF) or open slag bath furnace (OSBF) (Nicholas & Basirat, 2022b). There is also ample opportunity upstream, within mining operations, to tackle the increasing presence of gangue in iron ores and need for removal. Beneficiation processes for low-quality magnetite ores (Fe₃O₄) are advanced, whilst innovation is required for more abundant hematite ores (Fe₂O₃) and problematic goethite ores (FeO₂H) which do not possess advantageous magnetic properties. Whilst not a showstopper, iron ore quality is a key feasibility constraint for the H₂-DRI-EAF production route.

The green H₂-DRI route essentially utilises indirect electrification and copious amounts of cheap CO₂-free electrons underpin the business case. H₂-DRI-EAF electricity consumption is estimated at 3.5 megawatt hours per tonne (MWh/t) for ore-based production which is over 5-times greater than the scrap-based EAF route which consumed 0.67 MWh/t steel (Vogl et al., 2018). Whilst the DRI shaft furnace must operate continuously (Zare Ghadi et al., 2023), the production route offers high flexibility due to the ability to ramp-up/down low-temperature electrolyzers, utilise the EAF batch process, hydrogen and HBI storage, and a variable scrap charge. The H₂-DRI technology was successfully proven at pilot-scale in 2021 by HYBRIT, a Swedish partnership between iron ore miner LKAB, renewable energy producer Vattenfall, and steel producer SSAB (Åhman et al., 2018). Following their lead, many companies have made H₂-DRI project announcements. A commercial scale project in Northern Sweden is currently being constructed by H₂ Green Steel, which is expected to start production in 2026 and ramp up to 5 Mtpa of green steel by 2030 (H2GS, 2023). Project conditions, however, were ideal in Northern Sweden for project investment – high quality ore, cheap and abundant hydropower, government financial support – and business model transfer to the EU and further abroad is more challenging (Öhman et al., 2022).

2.1.5. Direct ore electrolysis is nascent technology with high impact factor

Direct electrolysis of iron ore, which separates iron ore into its constituent elements of iron (Fe) and oxygen (O₂) through the sole application of electrical energy, could be a pivotal near zero-emissions production route, however, the technology is immature and yet to be validated outside the laboratory.

In brief, electricity is applied to an anode and a cathode, which are immersed in an iron ore-containing solvent. This causes attraction between positively charged iron ions and the negatively charged cathode, as well as the negatively charged oxygen ions and the positively charged anode. If the electricity used is CO₂-free, green iron is produced with oxygen as the byproduct (worldsteel, 2021a). Electrolysed iron is pure (~100% Fe) so impurities will not need to be oxidised and removed via slag, but alloying elements must be added in a subsequent furnace (e.g., EAF) to achieve desired steel properties. Importantly, this technology circumvents the supply chain dependency on high quality iron ore as seen in the H₂-DRI route as a wide range of ore grades can be used, even those lower than BF-grade. The estimated energy consumption is 3.6 MWh/t steel, closely aligning to that of the H₂-DRI-EAF route (Cavaliere, 2019).

There are two main development arms: molten oxide electrolysis (MOE) which operates at 1600°C to produce liquid metallic iron, and low-temperature electrolysis (electrowinning) which operates at 50-100°C to produce solid metal. For MOE, a key technical challenge is developing electrolyte cells that can withstand temperatures over 1538°C (the melting point of iron) and uses affordable and readily available materials (Bailera, et al. 2021). Given continued investments, a pilot-scale project is foreseeable by 2030; in fact, Boston Metal expects a pilot plant to be operational by 2026 (Boston Metal, 2023). It also requires a continuous and stable supply of electricity as the process is not entirely flexible, and the produced hot liquid metal must be fed directly into downstream refinement processes. Advantageously, electrowinning is similar to processes already used to produce copper, nickel and zinc, and flexible, so energy-production system optimisation with variable renewable inputs is feasible. Despite the transferability of electrowinning technology from alternate metal production, challenges arise as iron oxide is difficult to dissolve in acid. Electra in the US have developed a two-step system which utilises an acidic iron salt solution in a proton exchange membrane electrolyser, and a subsequent anion exchange membrane electrolyser (Pham et al., 2022), which has attracted significant funding and expects a pilot plant to be operational by 2024 (ElectraSteel, 2023). In contrast to Electra's acid-based process, EU projects have explored the use of an alkaline electrolyte solution (Olsen et al., 2016). Hence, iron ore electrolysis may enable widespread direct electrification of steel production, however, the technology is still in its infancy.

2.2 Systems engineering approaches to steel decarbonisation

2.2.1 A systems-based, locational research agenda to investigate physical pathways to near zero-emissions

The clean energy transition presents the opportunity to reassess supply chain structures through space and time; “the geographies of a future low-carbon economy are not yet determined...a range of divergent – and contending – potential geographical futures are in play” (Bridge et al., 2013). Traditional steel production networks which rely on fossil fuels are not tied to the future near zero-emissions industry; with the necessary switch to renewables-based steel production, novel supply chains must be explored. To explore the most efficient and feasible flows of materials and energy from raw materials to markets, systems engineering tools can be utilised. These tools support holistic design of sustainable energy and production systems, from individual processes to global supply chains, and include lifecycle

assessments, material flow analyses, and system dynamics modelling. A key systems-based approach for assessing pathways for industrial decarbonisation is energy system modelling with integrated supply chain assessment. Following, one of the most powerful tools for solving complex problems with practical, integrated solutions is energy system optimisation modelling (Bazmi & Zahedi, 2011). Moreover, a locational, systems-based research agenda has emerged for industrial decarbonisation with energy system modelling at its core.

This research is guided by principles of industrial ecology, which values the inextricable relationships between society, the economy and the natural environment (International Society for Industrial Ecology, 2023). Through an industrial ecology lens, one can appreciate the circularity of material and energy flows, finite nature of resources, and variability in temporal and spatial scales of system components (Jelinski et al., 1992). Natural resource management and supply chain management are also closely related concepts, with the latter emphasising operations (Seuring, 2004).

System-based approaches play an important role in determining feasible and efficient decarbonisation trajectories, and thereby shaping investment priorities and influencing policymakers. Whilst this research focuses on physical decarbonisation pathways, others focus directly on policy-enabled pathways. Of note, policy levers for decarbonisation of the steel industry have been explored in the UK (Richardson-Barlow et al., 2022), EU (Vogl et al., 2021a) and global (Arens et al., 2021) contexts, with a focus on climate- and energy-centric strategies and carbon pricing. Approaches include demand side market creation, direct production subsidies (e.g., carbon contracts for difference), renewable electricity price guarantees, and carbon pricing schemes. Åhman et al. (2020) argued that national and regional policies are insufficient in driving global change, proposing international cooperation through green materials clubs as a more effective method to drive global decarbonisation and prevent carbon leakage. Robust qualitative approaches that inform how to deploy and sustain the growth of low and zero-emissions technologies can influence a wide range of stakeholders in the steel sector, especially policymakers, project investors, and standards organisations.

2.2.2 Sectorial technology-led roadmaps to near zero-emissions by 2050

A growing number of studies covering energy systems modelling have examined the technology-led pathways to 2050, providing a blueprint for industrial change. Important contributions include those developed by the Mission Possible Partnership (MPP, 2022), Science-based Target Initiative (SBTi, 2023), Net Zero Steel (NZS) Project (Bataille et al., 2021), International Energy Agency (IEA, 2021c), and One Earth Climate Model team (Teske et al., 2022). The key modelling inputs differentiating each study (some containing multiple scenarios) were the projected global steel demand (1.6-2.6 Btpa), scrap availability, allocated carbon budget (see Figure 2.4), and emissions reduction trajectory (see Figure 2.5). Methods differed in the spatial coverage, as well as the computational method; some utilised a bottom-up optimisation model where the objective function was to minimise costs whilst not exceeding the carbon budget, whilst others utilised top-down budget allocation with technology diffusion probability. The consistent short- to medium-term trend was a two-pronged approach whereby the majority of steel producers needed to reduce emissions incrementally, with a minority of ‘first movers’

investing early in near zero-emissions technology. Deep decarbonisation technology diffusion rates varied, but followed similar patterns; in 2050, the IEA forecasted that 53% of primary steel production will be CCUS-equipped processes, compared to 29% for H₂-based DRI-EAF and 13% for iron ore electrolysis-EAF, whilst MPP (carbon cost scenario) forecasted 36% CCUS-equipped processes, 25% H₂-based DRI-EAF, and 0% iron ore electrolysis.

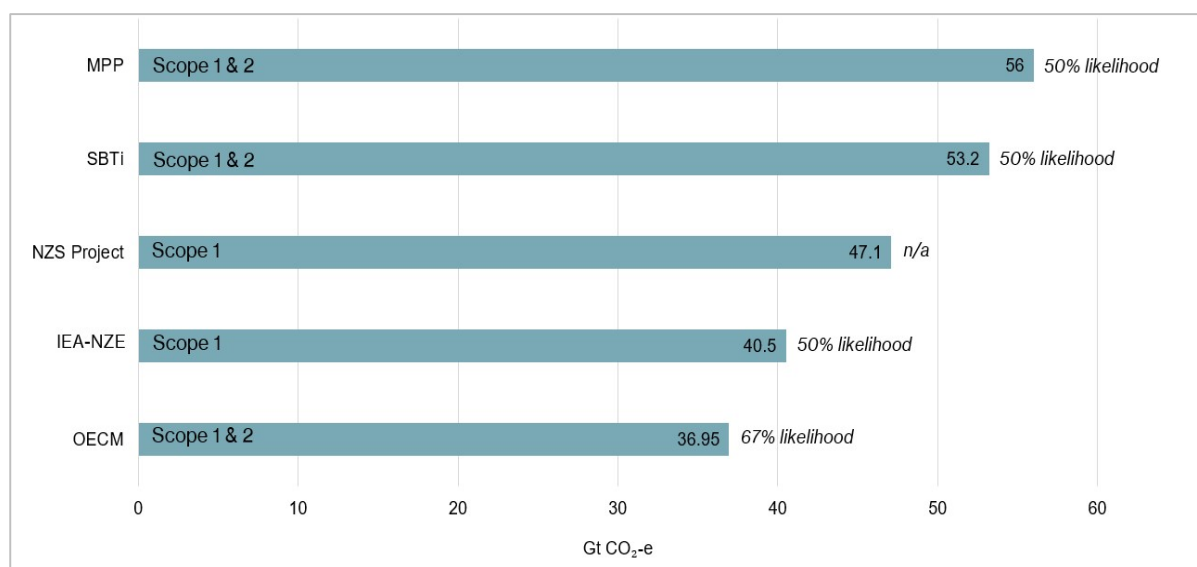


Figure 2.4 Comparison between key carbon budget estimations for the global steel sector in the 30 years from 2020 to 2050. Each method is unique, especially the chosen emissions boundary, and likelihood of keeping global warming to 1.5°C. The steel sector's budget is a portion of the global budget, which the IPCC have determined to be 400 Gt CO₂ for a 67% likelihood of achieving 1.5°C, and 500 Gt CO₂ for a 50% likelihood (IPCC, 2023).

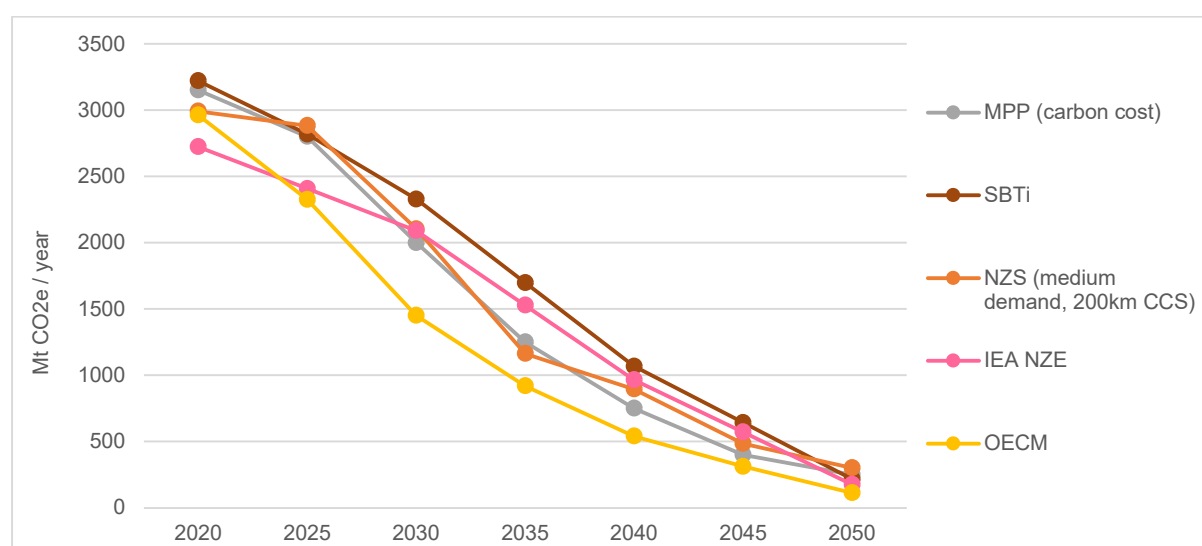


Figure 2.5 Comparison between 1.5°C-aligned pathways to near zero-emissions in 2050 for the global steel sector. Each method is unique, especially regarding the overall carbon budget, as well as scrap availability and steel demand forecasts.

Steel is a globally trade commodity and the sector is widely dispersed, calling for a globally aggregated transition roadmap to align decarbonisation strategies and multiply benefits. However, regional separation is essential to valorise the differing economic parameters, scrap availability and steel demand projections, as well as policies and regulatory frameworks, as provided in the models developed by the MPP and NZS projects. The distinction between decarbonisation agendas of developed and developing countries is also important; for example, Germany's net zero emission target year is 2045, whilst China targets 2060, and India 2070 (Climate Action Tracker, 2022). Following, regional and national technology-led roadmaps to near zero-emissions have been investigated specifically for the EU (Eurofer, 2019), UK (Griffin & Hammond, 2019), Sweden (Toktarova et al., 2020) and India (Gulia et al., 2023). In addition, China's short-term partial decarbonisation pathway was assessed through a top-down optimisation approach with a technology focus on BF-BOF phase out and increasing scrap availability (Li et al., 2023). These roadmaps are not predictors, but rather projections based on a plethora of techno-economic assumptions. They support understanding of the key levers for sectorial decarbonisation, including technology dependencies and consequent financial investments required. All long-term models reinforce that the pathway to near zero-emissions will not be driven by a single abatement measure - material efficiency, energy efficiency, hydrogen, electrification and CCUS will likely contribute in some capacity. There is also agreement that despite renewably powered EAF production being a feasible pathway forward, it will not suffice steel demand even under assumptions of reduced demand and increased material circularity. Nevertheless, to decarbonise the steel industry immense quantities of green electrons are necessary to substitute fossil fuels, which can be used to directly electrify processes, or indirectly, to produce green hydrogen.

2.2.3 Energy system modelling for steel production systems: from individual processes to complete supply chains

To switch the energy source in steel processing from fossil fuels to renewables, the business case must be convincing. Energy system modelling can be employed to investigate a range of techno-economic challenges, from matching VRE with inflexible operating processes, to determining the optimal locations of supplier and producer nodes in green H₂-based steel supply chains. Due to the locational research agenda, existing steel decarbonisation studies covering energy system modelling are grouped by spatial resolution – process/plant, nation/region, and supply chain – for discussion below.

At process level, analysis of green H₂-DRI production has dealt with the new dependencies between the steel and energy sectors, uncovering opportunities to improve process efficiency and reduce steel production costs. The steel industry is unique in its use of green H₂, not only as an energy source but for its essential chemical properties that enable iron ore reduction. Original contributions of the fundamental H₂-DRI chemical process were published by Vogl et al. (2018) for the Midrex shaft furnace (which requires external gas reforming), and Bhaskar et al. (2020) for the HYL-Energiron shaft furnace (where gas reforming is integrated in the shaft furnace), both providing mass and energy flows including CO₂ emission estimates. Krüger et al. (2020) and Müller et al. (2021) investigated the benefits of heat integration between DRI and high temperature electrolysis, the latter which also explored blended H₂/NG feed gas compositions in the transition to 100% H₂. The cost-minimised production of green

hydrogen is foundational to the cost-minimised production of green iron, and then green steel. Whilst some studies have treated H₂ as an external input, many have managed electrolysis internally as it can be coupled with DRI and EAF processes. Hydrogen-specific energy system optimisation studies are numerous, spanning production (Armijo & Philibert, 2020), to storage and transportation infrastructures (Moreno-Benito et al., 2017), and end-use pathways (Bellocchi et al., 2023). Ammonia, a key H₂ energy carrier, has also attracted attention, from process optimisation (Cesaro et al., 2021) to intercontinental transport routes (Salmon et al., 2021). Many of the lessons learnt are transferable to the steel sector: maximise process flexibility, utilise firm sources of power to balance renewables-dominated energy systems, integrate process buffers in the form of energy and material storage, and maximise shared infrastructure through colocation. Nevertheless, iron and steel production require focused process level research for the unique use of H₂ as iron ore reductant, sensitivity of metallurgical processes, and opportunities for process coupling, among others. More broadly, the steel sector's decarbonisation proposition is uniquely challenged by the scarce quality and quantity of iron ore and scrap resources, highly globalised supply chains (and hence susceptibility to carbon leakage), immense capacity of existing fossil-based assets with long campaign lives, and the sheer magnitude of steel consumed.

At national and regional level, studies have looked at the integration of renewables-based steel production at scale, with local resource availability considerations. Otto et al. (2017) quantified the energy demand requirements for a complete H₂-based German steel sector, comparing the energy demand and emissions abatement potential of grey H₂ (produced via SMR) and green H₂ (produced via electrolysis). Extending the geographical boundary to Germany and Scotland, Toktarova et al. (2021) investigated the cost implications of flexible DRI-EAF operation using H₂ and HBI storage, including hydrogen storage in lined rock caverns, and determined that approximately 20% reduction in steel production costs was achievable by matching process flexibility with VRE profile. Pimm et al. (2021) investigated the energy system requirements of H₂-DRI-EAF production in the UK, quantifying the optimal combination of generation and storage technologies, whilst Bhaskar et al. (2022) optimised H₂-DRI production in Norway, comparing a fixed electricity price against a variable (one-day ahead) price. The recurring conclusion was that competitive steel production costs were highly dependent on the sourcing of high-quality renewable energy (characterised by a high hourly capacity factor, as well as low daily and seasonal variability), which in turn drove down electricity and green H₂ prices.

At supply chain level, just a handful of papers have covered optimal green H₂-based iron and steel supply chain configurations. Gielen et al. (2020) introduced the concept of industrial relocation of energy-intensive industries to take advantage of high-quality renewable resources, and therefore low-cost renewable electricity, using Australia as the case study where land availability was also a crucial factor underpinning zero-emissions H₂ and HBI production potential. Following this industrial ecology framework, Wood et al. (2020) provided a case for green HBI and steel exports from Australia to Indonesia and Japan, and Trollip et al. (2022) highlighted the opportunity to export HBI from South Africa, a nation with iron ore and high-quality solar energy, to Europe, a region with negligible iron ore resources and high electricity prices. Toktarova et al. (2022) looked at the feasibility of supplying the Northern European steel sector with electricity, determining the cost-efficient spatial allocation of

electrified steel production capacity. Lopez et al. (2023) investigated five different supply chain configurations in Germany, Spain, and Finland, investigating the utility of H₂ and HBI imports from solar-rich trading partners of Morocco and Chile. Zooming in on supply chain enablers, some studies have also looked at regional technology diffusion dynamics: Pye et al. (2022) demonstrated the importance of considering H₂-DRI technology diffusion and regional spillovers which drive down costs and cumulative emissions (by about 13%), whilst Kushnir et al. (2020) carried out a technological innovation system study of the Swedish steel industry, highlighting the importance of coordinating technical infrastructure deployment and carbon policy alignment. Supply chain optimisation in steel decarbonisation literature has not been limited to the applications of renewable energy and green H₂. The viability of integrating biomass and carbon capture and storage across 30 integrated steel plants in the EU has been assessed, accounting for the biomass and CCS supply chains (Mandova et al., 2019). The role of forest biomass in abating fossil CO₂ emissions in the iron and steel industry has also been explored in Sweden, showing that biomass substitution targets are more influential than carbon prices (Nwachukwu et al., 2021). Moreover, whilst systems-based assessments within steel industrial decarbonisation literature are growing, the promising methodologies must be further developed to unpack efficient strategies to reach near zero.

2.2.4 Literature Gaps

Steel decarbonisation technology is advancing and gaining industry traction; simultaneously, the body of literature is growing that documents these advances and evaluates viable pathways forward. As explained previously, from the range of innovation areas being pursued for ironmaking, green H₂-DRI is the technology of highest maturity and near zero-emissions potential, despite CCUS-equipped processes often having higher shares in projected pathways to near zero 2050. Systems-based approaches including energy system modelling and supply chain assessments are effective methods of examining the industrial decarbonisation challenge and have been utilised by several studies in related literature, however, just a handful have focussed on renewables-based steel production networks and of those that exist, low spatial resolution and coverage is offered – a gap this thesis seeks to address.

More specific literature gaps can be identified for each of the key research chapters. Firstly (related to Chapter 3), at process level the existing studies of H₂-DRI-EAF production focus on the detailed thermodynamics and chemical processing steps, with some applications of optimisation modelling to matching VRE with industrial processes of varying flexibility. However, existing studies lack a broad geographical scoping of where optimal locations may exist. Effective supply-and-demand balancing mechanisms for industrial processes require locational adjustments. To fill this need, full appreciation of local renewable energy and iron ore resources across the diverse global landscape of present and potential future steel producers, and their impact on green steel market competitiveness, is explored in the first research chapter. Secondly (related to Chapter 4), the few existing studies that have explored steel industrial relocation and the transnational trade links focused on the business-enabling conditions, financial and policy levers, leaving a quantitative analysis gap. Whilst inspirational, what remains to be explored is a detailed assessment of energy utilisation efficiency of different supply chain configurations

and a corresponding techno-economic analysis within the projected decarbonisation timeline. Hence, the second original research chapter looks to fill this gap with a spatially granular computational approach that critically evaluates into the energetics and economics of prospective supply chain configurations. Thirdly (related to Chapter 5), supply chain optimisation, which investigates the movement of energy and mass across time and space, is absent in steel decarbonisation literature. Existing sectorial transition roadmaps lack a spatially granular understanding of resource constraints – iron ore, renewables, scrap, land – which acutely affect feasibility. Too, most assume technology conversion within existing steel plants rather than greenfield project establishment, which limits the potential. The final chapter seeks to fill these literature gaps by developing a geospatial explicit supply chain optimisation model for economies in transition.

A closing window of opportunity exists to make the investments required to keep steel emissions aligned to a 1.5°C-aligned trajectory given the long fossil-based asset lifetimes and long renewables-based project timelines (which limit usual investment milestones and the pace of change). It is necessary and timely to explore advantageous supply chain configurations that diverge from present day dynamics, through a quantitative, spatially granular approach which untangles the feasibility of technological solutions and transition strategies. Supply chain optimisation, where the movements of mass and energy from raw materials to markets are evaluated, are currently rudimentary in steel decarbonisation literature but deserve more attention given their importance in uncovering holistic energy efficiency, emission reductions and cost-competitiveness. Hence, the new map of global green steel production is explored in this thesis.

Chapter 3. Global Co-located Green Hydrogen-Based Steel Opportunities

Overview

This chapter presents the following published article: Devlin, A., Kossen, J., Goldie-Jones, H., & Yang, A. (2023). Global green hydrogen-based steel opportunities surrounding high quality renewable energy and iron ore deposits. *Nature Communications*, 14(1), 2578. <https://doi.org/10.1038/s41467-023-38123-2>. The corresponding Supplementary Information is contained within Appendix I.

Among all authors who contributed to the research, A.D. conceptualised the study, developed the models, analysed the results, and wrote the manuscript, A.Y. supported with the conceptualisation, provided feedback on the modelling, and revised the manuscript, J.K. supported the machine learning modelling, and H.G.-J. supported data collection and analysis. The GAMS (General Algebraic Modelling System) optimisation code developed by A.D. in this study is available online (<https://figshare.com/s/92ed30035b61fd174d93>), in addition to the machine learning code developed by both A.D. and J.K. (<https://figshare.com/s/a3849465ee2e09744876>).

This first piece of original work harnessed the opportunity to redesign steel supply chains around high-quality renewable energy (i.e., with a strong capacity factor and limited intermittency for combined solar and wind sources) and iron ore (i.e., low gangue content and high Fe-content). The market competitiveness of one of the widely considered decarbonisation routes for primary steel production – green hydrogen-based direct reduction of iron ore followed by electric arc furnace steelmaking (H₂-DRI-EAF) – was investigated through a local lens but at global scale. Very high temporal and spatial resolution was obtained through facility-level optimisation which modelled 1 Mtpa of green H₂-based steel production, repeated in 44 regions of 17 of the most important iron ore-producing countries, then expanded to over 300 locations using machine learning applications. By internalising hydrogen, iron and steel production within the facility-level analysis, the cost-reduction benefits of matching VRE with process flexibility could be comprehensively explored. The simplest supply chain was utilised whereby iron ore mining, hydrogen production, ironmaking and steelmaking were all co-located, forming a baseline for future supply chain complexity. By focusing on greenfield projects and thereby removing the influence of existing assets, every location could be compared equally. This methodology allowed the global potential of green H₂-based steelmaking using local solar, wind and iron ore resources to be mapped. This evaluation of H₂-DRI-EAF co-location was an important first step before investigating more complex supply chain configurations.

3.1 Introduction

In this study, we provide a baseline assessment of the global potential of renewables-powered steel production using green H₂-DRI-EAF technology, where the entire supply chain is co-located within the iron ore mine's vicinities. Taking into account the VRE and iron ore supply challenges, this work particularly considers the geographical distribution of local resources. The key question of interest is, across all the major iron ore deposits, to what extent these locations show promising green H₂-based steel economics. Answering this question will identify regional opportunities and inform the future design of more sophisticated supply chains for regions which need to go beyond the simple co-location strategy, involving trade of ore, renewable energy (RE) products, and/or intermediate steelmaking products, such as HBI.

The main part of the study consists of two steps, as illustrated in Figure 3.1. In the first step, a techno-economic optimisation model was developed for localised green H₂-based steel production adjacent to iron ore deposits, based on regional RE profiles at hourly temporal resolution. The optimal capacities of all key technical components (energy supply and storage, DR shaft furnace, EAF) were determined for a H₂-DRI-EAF steel facility with 1 Mtpa output, a reference scale chosen based on the range of scale for EAF steelmaking (0.3-3 Mtpa, Renda et al. (2013)) and current DR ironmaking nominal capacities (0.4-2.5 Mtpa, GEM (2022)). Applied to three deployment (hence technology advancement) timelines (2030, 2040, 2050) combined with different levels of scrap steel (0%, 25%, 50%), the model was solved for 44 regions in 17 important iron ore producing countries. For each region, the cost of obtaining iron ore suitable for DRI based on the national iron ore quality data was further estimated and combined with the labour cost and the output of the optimisation model for steel production, to establish the overall cost of green H₂-based steel. Due to limited global ore petrology data availability, Fe content was the single indicator used for iron ore quality. Solar and wind were chosen as the core renewable energy resources for analysis as they are available in all studied locations, and are predicted to deliver 70% of global electricity generation in 2050 (IEA, 2021c). In the second step, outputs from the optimisation model were processed using machine learning techniques to derive a green H₂-based steel investment model, which, thanks to its much higher computational efficiency, enabled expansion of the global assessment to >300 deposits in 68 countries.

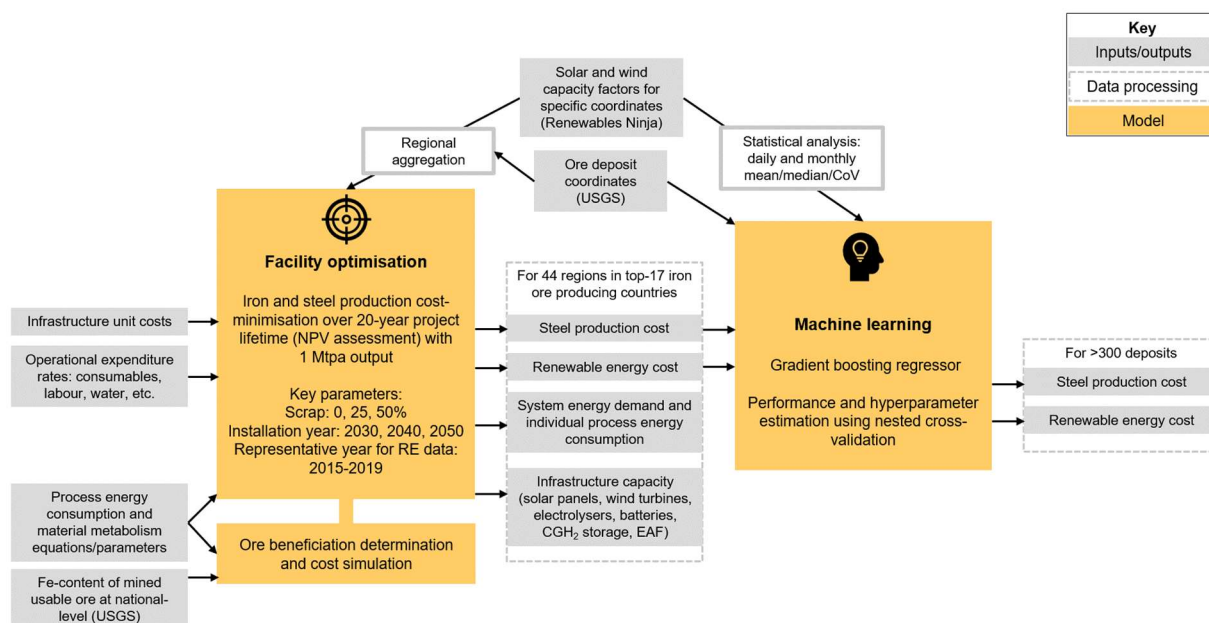


Figure 3.1 Schematic of methodology for the global green H₂-based steel production assessment.

Islanded (100%) RE supply, although ensuring nearly zero carbon emissions, exhibits intermittency and variability which can be managed using energy storage and/or oversizing flexible production plant (Armijo & Philibert, 2020; Chen & Yang, 2021). For comparison, we also assessed H₂-DRI-EAF plants powered by grid electricity, which offers stable energy supply. We assumed that the grid power's carbon footprint was dependent on the forecast power mix and that electricity was charged according to current industrial tariffs, for the sake of assessing conditions for competitive steelmaking and providing recommendations for electricity market reform. The economic and carbon emission perspectives of both schemes were evaluated with reference to the conventional BF-BOF route. Finally, the energy, water and land use implications and further challenges that the H₂-DRI-EAF route needs to address for large-scale implementation were considered.

Through combined use of optimisation and machine learning, we demonstrate in this study that for market competitiveness, it is important especially in the short term to locate flexible green-H₂ based steelmaking in favourable locations, commonly characterised by strong and reliable solar, fair supplementary wind, and high-quality iron ore. If coking coal prices remain high and projected cost reductions are realised for electrolyzers, solar panels and wind turbines, the majority of locations could become competitive against the fossil-based BF-BOF route by 2050. By illustrating the global map of projected solar and wind-powered steelmaking costs, we show that green steel investment decisions must revolve around climatic and geospatial factors.

3.2 Methods

3.2.1 Description of the steelmaking system

Green H₂-DRI-EAF steel production with various shares of scrap (0%, 25% and 50%) were modelled, alongside 2030, 2040 and 2050 project installation years. The co-located supply chain spanned from iron ore mining and renewable energy generation to the production of semi-finished steel products via continuous casting (see Figure 3.2). Whilst key aspects are described in this section, refer to the Supplementary Methods (of Appendix I) for further details.

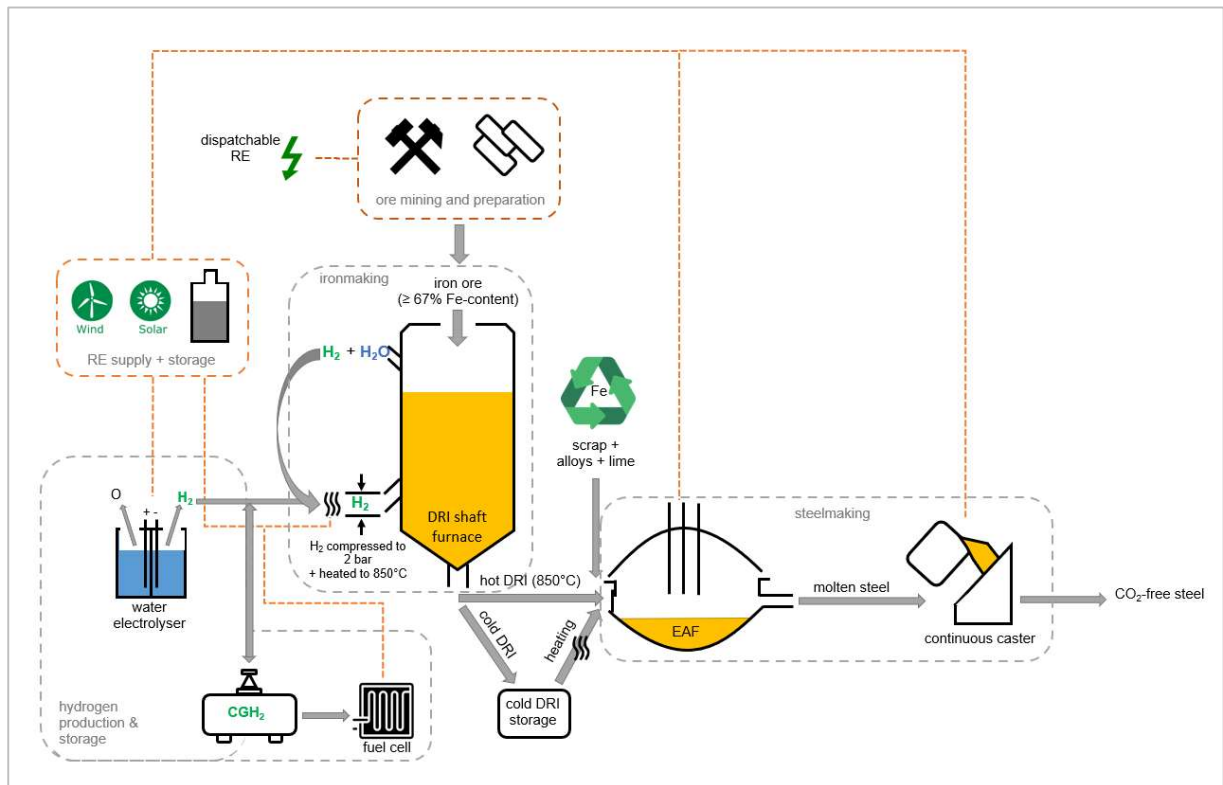


Figure 3.2 The modelled integrated green H₂-DRI-EAF steel production system. The overall production system consisted of five sub-systems: RE supply and battery storage, hydrogen production and storage, iron ore mining and preparation, ironmaking, and steelmaking. All processes are co-located and the solar and wind energy supply is fed to all other sub-systems, either directly or indirectly via battery or hydrogen storage.

RE supply and battery storage. Solar and wind resources directly energised electrical processes, and indirectly energised chemical processes via green hydrogen production. Storage of electrical energy was enabled through lithium-ion battery integration (85% charge/discharge cycle efficiency) or compressed gaseous hydrogen (CGH₂) converted via the fuel cell to electrical energy (~40% round-trip efficiency). A lithium ion battery was selected for electricity storage due to its relative high efficiency, prolonged cycle life (up to 10,000 hours at 100% depth of discharge) and intermediate self-discharge rate (5-8% per month at 21°C) in comparison to other battery technology (IEA and IRENA, 2012; Vega-Garita et al., 2019).

Hydrogen production and storage. Green hydrogen is produced through renewable-powered water electrolysis. Multiple electrolyzers are in development with key differences in the current/projected energy efficiency, unit cost, cold start time and lifetime. Low-temperature (80°C) alkaline technology is mature with reasonable dispatchability to respond to variable renewable energy inputs (IRENA, 2021), and hence was selected for this study. Due to electrolyser modularity, electrolyser capacity was treated as a continuous variable. CGH₂ stored aboveground in steel tanks at 200 bar pressure was incorporated into the energy system as both a H₂-buffer (pre-DRI) and energy store when combined with fuel cell stacks. Although underground CGH₂ storage may be preferred on an energy efficiency basis for seasonal storage (lower pressures required), a storage option with rapid charge/discharge rates was prioritised (storing H₂ in geological formations, an option that may become relevant for large-scale implementation).

Iron ore mining and preparation. Iron ore is a naturally occurring geological resource from which metallic iron (Fe) can be extracted, most commonly present as hematite (Fe₂O₃) or magnetite (Fe₃O₄) with varying levels of Fe-content (global average of 62%) (U.S. Geological Survey, 2022). The ore is then processed to produce a marketable product of specific physical form (lump, pellet, fines) and Fe content (DR-grade ore ≥ 67% Fe). Beneficiation, a process whereby gangue material is removed and Fe concentration increased, is proceeded by pelletisation to produce DR-grade ore. Depending on the degree of beneficiation required, crushing, screening, and grinding processes are utilised in conjunction with gravity or magnetic separation. Whilst very high quality deposits can be mined and used as lump, DRI shaft furnaces are technically constrained to a lump-to-pellet ratio of 3:7 to prevent ore clustering (Linklater, 2021).

Ironmaking. DR-grade iron ore is reduced by H₂ at a minimum consumption rate of 50 kg H₂/t DRI and metallisation rate of 94% (Kirschen et al., 2011). Prior to injection into the shaft furnace, H₂ is heated to 900°C (gas acts as reductant and heat carrier) and compressed to 2 bar (to overcome furnace pressure drop). DRI operations are generally continuous with minimum load variation to ensure uniform internal reduction kinetics (Najmi et al., 2019). The outputted sponge iron can be fed directly to the EAF (as hot-DRI at 850°C), stored on site (as cold-DRI) for later re-heating and EAF charging, or modified into a more stable product as HBI (Midrex, 2018). Since iron and steelmaking are co-located in this study, only hot-DRI and cold-DRI are utilised. Hydrogen direct reduction processing was based on Vogl et al. (2018), whilst the energy and H₂ requirements were determined using Aspen Plus simulation.

Steelmaking. EAFs are charged with DRI, scrap, alloys, and lime, and consume carbon electrodes to produce molten steel at 1600°C. Metal yield is inhibited by DRI gangue content; impurities can be removed via EAF slag which is stimulated by slag formers such as lime fluxes, although this is an energy-intensive process and impurities are best dealt with during DRI. Increasing the scrap charge will reduce slag demand, lime demand and EAF energy consumption (Kirschen et al., 2021). The EAF operates in batch mode and often a single steel plant will have multiple EAFs of various capacities. The model considered a 60-minute tap-to-tap time for each batch; for simplicity, EAF operation was treated as a continuous variable.

3.2.2 Location selection and geospatial characterisation

The top-16 iron ore producing countries were selected for analysis, constituting 98% of ore production (by output quantity) (U.S. Geological Survey, 2022), with the addition of Guinea, a nation with high quality ore (65.5% Fe) which has not yet been extracted (Rio Tinto, 2018). A country was split into multiple regions when the national deposits were dissimilarly located (classified as when the standard deviation of latitudes and longitudes exceeded 1°), totalling 44 regions (see Table S3.5).

Solar and onshore wind potential was determined using Renewables Ninja, which provided data for each of the 8760 hours across the five selected historical years: 2015-2019. RE data was extracted at coordinate-level for each ore deposit, then regionally aggregated across multiple deposits. Despite publicly available records of the exact coordinates of each iron ore deposit, ore production and reserve data was only available at national level (U.S. Geological Survey, 2022). The applied Fe content was determined by current extracted ore characteristics (as opposed to the reserve characteristics) as this more accurately reflected the economic resource and mine operation feasibility (refer to Table S3.6 for key geospatial dataset details).

For simplicity, ore cost adjustments were modelled as a function of Fe-content. DR-grade lump ore is a premium product due to the very high reserve grade requirements ($\geq 66\%$ Fe), and DR-grade pellets due to the additional energy (communion, concentration and pelletising) and material inputs (binder). Based on top-down accounting from the 62% Fe market reference price of \$100/dry metric tonne (dmt) (10-year average, World Bank Group (2022a)), ore production costs were assumed to be \$60/dmt for DR-grade lump, and an average \$100/dmt for DR-grade pellets (Equation 3.1). An extra \$10/dmt was added to Sweden's site costs due to underground operations and consequent drilling and blasting requirements at Kiruna, the dominant national mine. Ore preparation energy demand was calculated alongside that of iron and steel production (see Tables S3.7 and S3.8 for mass loss rates and process specific energy consumptions).

Equation 3.1 DR-grade pellet cost (\$/dmt)

$$C_{DR\ pellet} = 60 + 40 * \frac{Fe_{global}}{Fe_{national}}$$

Fe_{global} = average global Fe content, 62%

$Fe_{national}$ = Fe content of extracted ore(t)/total extracted ore (t)

Apart from these geospatial features, scrap prices and steelworker wages were regionally differentiated (refer to Tables S3.17 and S3.18, respectively). Scrap steel unit prices were regional variables based on the export price, excluding Turkey (dominant global scrap steel importer) for which import price was used (HS 720429 Waste or scrap, of alloy steel, other than stainless from UNComtrade (2021)).

3.2.3 Optimisation of islanded RE-driven steel making facilities

A linear programming optimisation model of the 1 Mtpa green H₂-based steel production facility was developed and solved using GAMS. The model pertained hourly resolution over a characteristic year and was optimised for lowest cost using the CPLEX solver. The objective function (Equation 3.2) was to minimise the steel plant's annualised costs ($Cost_{ann}$), covering both capital expenditure (CAPEX) and operational expenditure (OPEX), given resource consumption parameters (see Table S3.10) and cost parameters (see Table S3.11) of the steel production process. The ore sub-system was an externally managed parameter; the quantity of ore required was a function of the steel scrap fraction and extracted ore Fe content. A Net Present Value economic assessment (Equations 3.3-3.10) was conducted over the 20-year project lifetime given a discount rate of 8%.

For all 8760 hourly timesteps across a year, the model determined the flow of energy to production, storage, or curtailment, which defined overall process capacities and production costs. Each model was run for a given location and RE input year (to consider inter-annual variability) over 9 loops for all combinations of project installation year (2030, 2040, 2050) and scrap input (0%, 25% and 50%). Over the two modelled decades, maturing RE technology (solar panels, wind turbines, li-ion batteries, electrolyzers, and fuel cells) benefitted from cost reductions and efficiency improvements (refer to Table S3.9). Although up to 100% scrap charge can be enabled in the EAF, 50% was chosen as the maximum charge in alignment with the maximum forecasted portion of secondary steel production towards 2050 (Stefan Pauliuk et al., 2013). The principal case for analysis was without scrap since it provided a direct comparison to the conventional BF-BOF route and removed instable scrap price influences. All costs are presented in USD, 2020 dollars.

The decision variables surrounded scheduling and capacity planning of each production unit, more specifically: (i) energy infrastructure capacity (solar panels (MW), wind turbines (MW)), (ii) production infrastructure capacity for flexible processes (electrolyzers (MW), CGH₂ storage (t), battery storage (MWh), EAF (t), continuous caster (t)), (iii) electricity storage medium (li-ion batteries (MW of 4-hr batteries) or CGH₂ storage (t) combined with fuel cells (MW)), and (iv) hot- or cold-DRI feed (t) to the EAF. The primary constraints were 1 Mtpa steel production and operation using a completely islanded energy system (zero dispatchable power integration). Water and land constraints, as well as carbon-intensity, were considered as systems enablers/disablers but not accounted for in the NPV analysis (water accounts for about 1% of total LCOS, as shown in Chapter 4). Whilst LCOS at site was the primary economic metric, transport costs to the nearest port were included for free on-board (FOB) costs and then marine transportation to Qingdao, China, for combined cost and freight (CFR) to the largest demand centre (see Table S3.12 for freight rates). Marine transportation was assumed to be powered by green NH₃ and solid oxide fuel cell combined with an electric motor.

Equation 3.2 Objective function

$$\text{Minimise: } Cost_{ann} = CAPEX_{ann} + OPEX_{ann}$$

Equation 3.3 Annualised CAPEX

$$CAPEX_{ann} = f^{CR} * (CAPEX_{production} + CAPEX_{storage} + CAPEX_{energy})$$

Equation 3.4 Capital recovery factor

$$f^{CR} = \frac{r(1+r)^n}{(1+r)^n - 1}$$

Where f^{CR} denotes the capital recovery factor, r represents the real discount rate (8%) and n denotes the project lifetime (20 years).

Equation 3.5 CAPEX of iron and steel production infrastructure

$$CAPEX_{ProductionPlant} = \sum_i (capacity_i * unit\ cost_i)$$

Where i denotes H₂ heater, DR shaft furnace, EAF and continuous caster.

Equation 3.6: CAPEX of hydrogen production infrastructure

$$CAPEX_{Electrolysers} = capacity_{electrolysers} * unit\ cost_{electrolyser}$$

Equation 3.7: CAPEX of renewable energy production infrastructure

$$CAPEX_{RE} = C_{solar} + C_{wind}$$

Equation 3.8: CAPEX of energy storage infrastructure

$$CAPEX_{EnergyStorage} = \sum_j (capacity_j * unit\ cost_j)$$

Where j denotes compressor (200 bar), CGH₂ storage vessel, fuel cells, and batteries.

Equation 3.9: Annualised OPEX

$$OPEX_{ann} = \sum_j (consumption_j * unit\ cost_j) + O_{mnt}$$

Where j denotes consumables (iron ore, scrap steel, lime, alloys, graphite electrodes) and labour.

Equation 3.10: Operation and maintenance OPEX

$$OPEX_{O\&M} = 0.02 * (CAPEX_{ProductionPlant} + CAPEX_{Electrolysers} + CAPEX_{RE} + CAPEX_{EnergyStorage})$$

3.2.4 Modelling the grid-based system and BF-BOF route

To investigate the relative cost competitiveness of various renewable energy systems, “variable-load islanded” was compared to “continuous-load grid” for 1 Mtpa green H₂-DRI-EAF facilities (without scrap charging). For the grid-based system, steel costs were differentiated at country-level by current industrial electricity tariffs (refer to Table S3.13) and projected grid carbon intensities (Knobloch et al., 2020). For islanded green H₂-DRI-EAF production, CO₂ emissions were also calculated and carbon prices applied, however only for the renewable energy system. 40g and 10 g CO₂/kWh for utility-scale solar panels (Burkhardt et al., 2012) and wind turbines (Dolan & Heath, 2012), respectively, were assumed. GHG emissions from electrolyzers, and iron and steel production facilities were not considered, as they were in the grid-powered production systems, due to negligible contributions. Projected carbon taxes were applied according to the IEA (2021e) net zero scenario and economy classification: advanced (Australia, Canada, Sweden, and the US), major emerging economies (Brazil, China, Russia, South Africa) and developing economies (Chile, Guinea, India, Iran, Kazakhstan, Mexico, Peru, Turkey, Ukraine), equal to \$250, \$200 and \$55/t CO₂ in 2050, respectively (refer to Table S3.16).

Both H₂-DRI-EAF systems were compared to the conventional BF-BOF route, with unique production costs for each country based on data from Transition Zero (2022) (see Table S3.15). National carbon-intensities of BF-BOF production were given by Hasanbeigi and Springer (2019), with economy-wide averages (weighted according to steel output) utilised for unspecified countries: 1.7, 2.3 and 2.6 t CO₂/t steel for advanced, emerging and developing, respectively (see Table S3.14). The marginal abatement costs were also calculated for both decarbonised steel routes, that is the minimum carbon price required to equalise BF-BOF costs.

It is necessary to acknowledge that once the energy system is decarbonised, some minor process emissions will remain within the green H₂-DRI-EAF route due to lime (28 kg CO₂/t steel), graphite electrodes (6 kg CO₂/t steel) and fossil-based carbon injection into EAF (17 kg CO₂/t steel) (Marcos et al., 2019). The decarbonised production route that removes carbon from the direct reduction of iron, however, also removes the necessary carbon source in the EAF to produce the C-Fe alloy that is steel (depending on the steel quality, C content in steel ranges from <0.3 – 1.5%). In absence of C-containing DRI, carbon can be injected into the EAF. Biogenic carbon (biochar, produced via torrefaction or gasification) can be used instead of coke at a rate of 12 kg/t steel (compared to 8 kg/t steel for coke), procured at a price dependent on the biomass cost but may be approximated at 235 \$/t, equal to less than \$3/t steel (Marcos et al., 2019). If biochar is used in place of coke for essential steel alloying, total process emissions can be reduced to 34 kg CO₂/t steel (1% of the BF-BOF route's emissions).

3.2.5 Building the machine learning model

ML was utilised to develop a rapid green H₂-based steel assessment tool, enabling cost projections for >300 locations (covering 68 countries) in less than a second. This was a significant timesaving considering the GAMS optimisation model's computational processing time of 3 hours (on a machine with Intel i7-8665U CPU and 16 GB memory of RAM running Windows 10) for a given location and RE

input year. Gradient-boosted regression models from the scikit-learn toolkit (Pedregosa et al., 2011) were fitted to directly predict two targets: levelised cost of renewable energy infrastructure (RE cost), and steel (LCOS, excluding ore and labour) for green H₂-DRI-EAF steel production without scrap charging in a 1 Mtpa facility. The ML algorithm learned from 675 data points: 45 regions modelled over 5 renewable energy input data years and 3 installation years. Note that New Zealand was the 45th region added to the 44 previously optimised regions to ensure the largest range of latitudes were covered in the input dataset. To determine the overall LCOS, statistical RE data from 2019 was used as features to project the machine-learned LCOS (excluding ore and labour), with separately computed costs of DR-grade ore and labour added.

Regression analysis accuracy relied on detailed characterisation of the renewable energy availability and intermittency at a specific location (becoming the features of the ML model). Renewable energy statistics were computed, encompassing the mean, median, and coefficient of variation (CoV) of the hourly and monthly capacity factors (CF). A multicollinearity analysis was undertaken using hierarchical clustering to remove redundant predictors, thereby preventing issues when interpreting feature importance.

A gradient boosting regressor was selected for ML as an additive model (i.e. sum of multiple simple models) that uses decision trees to accurately predict continuous values. Nested cross-validation (CV) was applied to estimate the generalisation performance (R^2 value) of the model and select optimised hyperparameters (which control the learning process). Since the regressor's purpose was to model novel locations, the key metric to maximise was the performance of regions not included in the training set. Nested CV involved a series of train/validation/test set splits where data was split into 17 folds such that each fold contained data from a single country. A set of countries were then selected as suitable for testing which excluded extreme regions that we did not expect the model to generalise to. For hyperparameter selection, we searched exhaustively over the Cartesian product of: (i) the learning rate, selected from [0.01, 0.1, 0.5], (ii) the maximum depth of the tree, selected from [3, 5, 10], and (iii) the number of estimators, selected from [100, 5000, 10000]. To obtain the final model, we set the hyperparameters to those that were selected most often in the inner CV and trained the regressor on the entire data set.

3.3 Results

3.3.1 High-quality renewables and ore for low-cost green H₂-based steel

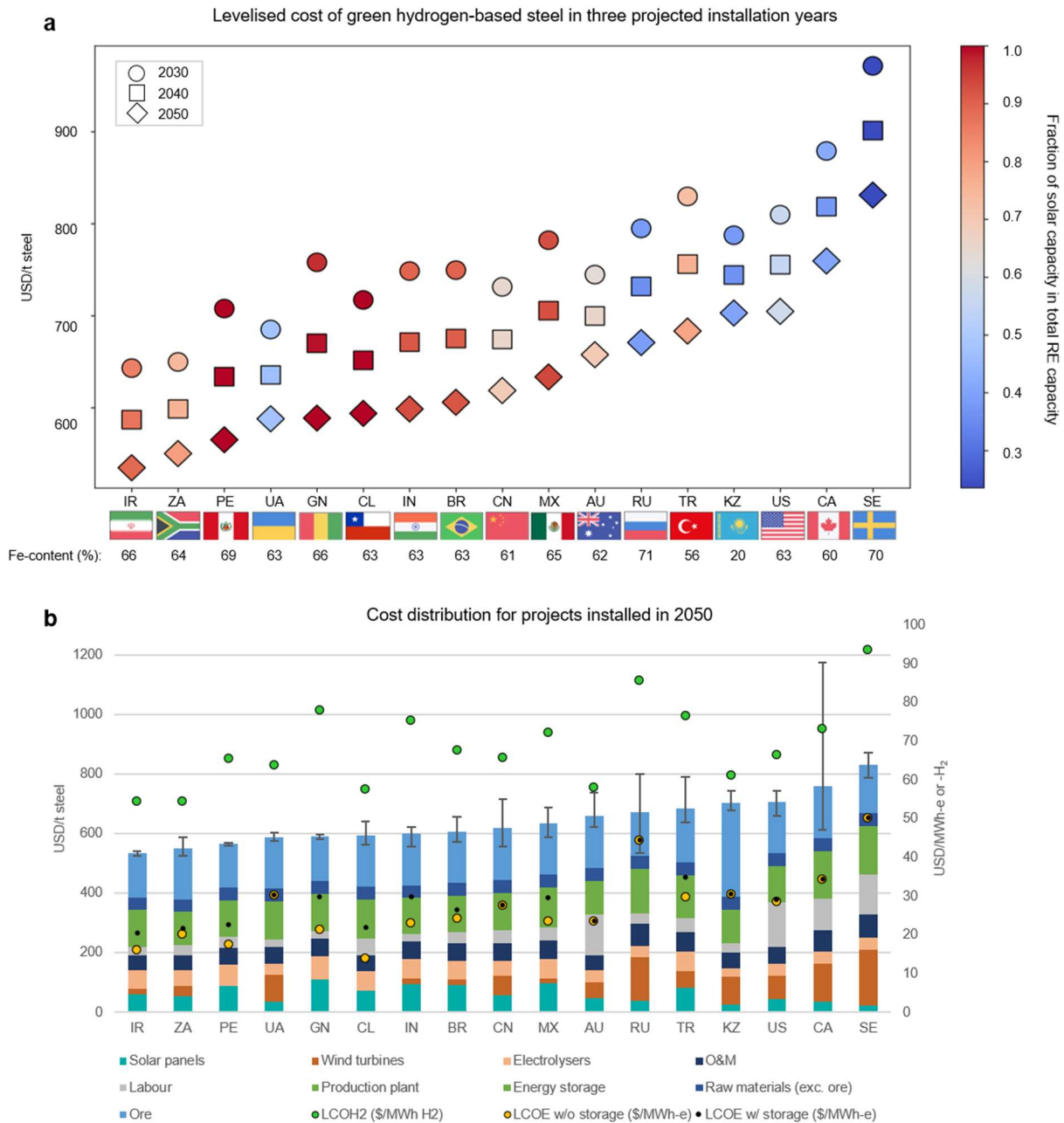


Figure 3.3 Optimisation results of H₂-DRI-EAF steelmaking with islanded RE supply (0% scrap). (a) Cost ranking of 17 countries over three projected years - 2030, 2040 and 2050. (b) Decomposition of the LCOS for each country for projects installed in 2050, plotted against the production system's LCOE and LCOH, with error bars showing LCOS interannual and inter-regional variation. Canada has an especially large error bar due to the variance in solar and wind energy across the large land mass where various iron ore deposits are distributed. Costs were obtained by averaging the results of optimisation runs using five different years of historic VRE data, and for a country with multiple iron ore deposit regions, cost figures at the country-level were obtained by averaging the regional results.

Our modelling of green H₂-based steel production, powered by islanded RE systems (solar and onshore wind) and localised at the iron ore mine site, projected LCOS in the range of \$535-972/t without scrap charging, as illustrated in Figure 3.3a. By 2050, the LCOS range dropped to \$535-\$831/t, with LCOH from \$1.63 to 2.80/t and LCOE (calculated based on energy consumed for steelmaking) from \$16 to 50/MWh, as shown in Figure 3.3b. Costs varied according to the region (affecting RE potential, iron ore quality, and workforce wages) and project installation year (affecting emerging technology unit costs and electrolyser efficiency). Favourable locations were solar-dominant in RE infrastructure albeit with some wind capacity to balance the diurnal profile; in 2050, the solar portion of RE capacity in the most favourable locations, being Iran, Peru, South Africa and Chile, were 89%, 100%, 80%, and 100%, respectively. Strong solar power potential with minimal seasonal variation allowed the production systems to profit from cheaper unit costs for solar PV panels compared to wind turbines (\$327/kW and \$835/kW, respectively, in 2050 (International Renewable Energy Agency (IRENA), 2019)) and reduce electrolyser oversizing and/or storage requirements. Across all cases, most energy storage costs were allocated to CGH₂ (mean 91%) with some electricity storage in batteries to manage RE variability; on average, 50% of produced H₂ was stored temporarily as CGH₂ whilst electrolyzers and EAFs were oversized by factors of 2.3 and 1.3, respectively. Affordable green H₂-based steel production was correlated to lower energy- and land-intensity.

Whilst the islanded energy supply has considered only locally available wind and solar resources, which represent the RE types that are most likely to dominate the growth of RE capacity in most countries in the next few decades, contributions from continuous and controllable zero carbon energy sources, i.e. hydropower (very important for countries such as Sweden and Brazil) and nuclear may play a critical role in competitive green H₂-based steel production. Although these alternate energy sources are not considered in the islanded case, they are reflected in the evolution of national energy mix in the grid-based case presented later.

As illustrated in the cost breakdown of Figure 3.3b, renewable energy capacity was more influential than iron ore Fe-content for cost performance, yet DR-grade ore beneficiation requirements challenged profitability. For example, Russia was disadvantaged by poor quality solar and mediocre wind resources, which high-quality ore (71% Fe-content) was able to only partially offset, resulting in low market competitiveness. By sensitivity analysis, a 10% change in ore costs caused an average 3% change in LCOS across all sites. If the ore quality was too low, however, beneficiation requirements would significantly increase production costs. In Kazakhstan, where the renewable energy supply is of reasonable quality thanks to its strong wind resources (as reflected in the LCOE and LCOH) but where ore is mined at extremely low quality (20% Fe-content, well below the global average of 62%), beneficiation requirements were immense and the DR-grade pellet premium tripled the average (from \$40/t to \$122/t ore); total ore cost accounted for 45% of steel production costs, well above the 27% average. Whilst Kazakhstan represents an extreme case, in general, current economic ore resources serve the BF market and may prove unprofitable for the DR iron-making market with enhanced quality requirements.

3.3.2 Market competitiveness achievable in the near term for ideal locations

The green H₂-DRI-EAF production route may be cost-competitive with the BF-BOF in favourable locations in the next decade, and for most locations towards 2050. The projected costs for green-hydrogen based steel produced at iron ore mine sites are plotted against current BF-BOF costs in Figure 3.4a. BF-BOF operational costs in 2021 ranged from \$621-\$782 per tonne in the selected locations, a steep increase from 2020 (\$428-\$547/t) due to a surge in commodity prices - notably metallurgical coal and iron ore (Transition Zero, 2022). Whilst there is uncertainty in projected commodity prices and market dynamics, increasing fossil fuel prices and decreasing renewable energy costs will increasingly favour the green-hydrogen based steel production route. Although, metallurgical coal prices may decrease if H₂-DRI achieves significant market share. With reference to the BF-BOF costs at the level of 2021, it was projected that in 2030, a number of studied regions will see market competitiveness (i.e. <\$782/t) of green H₂-based steel powered by islanded solar and onshore wind (without scrap charging nor a carbon tax). To reduce the cost premium between fossil-fuelled and renewables-based production, which would be significant if BF-BOF production costs returned to 2020 levels, carbon pricing mechanisms would become essential.

EAF scrap charging can drive cost benefits, so long as contaminants are controlled to avoid affecting steel quality and product lines. Scrap addition generally reduces the LCOS, however, benefits lessen over time with cheaper renewable energy. In 2030, a clear relationship is evident between scrap addition and production costs, a result of the reduced DRI requirement and EAF energy demand (25% scrap addition drives 5% cost reductions, 50% scrap addition drives 9% cost reductions). Towards 2050, however, scrap is less influential in reducing production costs due to the decrease in RE costs which makes green DRI cost-effective and comparable to scrap (50% scrap addition drives 2% cost reduction). Scrap charging into the EAF favoured countries with cheap scrap: China (\$212/t scrap), Sweden (\$355/t), Brazil (\$380/t) and Chile (\$387/t), whilst disadvantaging those with expensive scrap: Russia (\$624/t), Ukraine (\$534/t) and Canada (\$472/t). Whilst scrap addition may aid in cost reduction it cannot be relied upon as supply is constrained by historical steel consumption rates and lifetimes of in-use steel stocks. In addition, BF-BOF production similarly benefits from the inclusion of scrap.

Despite green hydrogen-based steel production generally consuming far less energy than the BF-BOF route (see Figure S3.2), the switch in dominant energy source from thermal to electrical requires optimisation of the renewable electricity system and minimisation of supporting infrastructure. Whilst energy represents 8-20% of BF-BOF production costs (Transition Zero, 2022), in the green H₂-DRI-EAF route, the renewable energy system (solar panels, wind turbines, electrolyzers) occupies 21-33% of total costs in 2050 (27-41% in 2030). Over the two modelled decades, average costs of projects installed in 2040 and 2050 dropped by 8% and 16% (compared to 2030), respectively, in line with long-term projections of reduced unit costs for RE infrastructure. Accordingly, the average LCOE and LCOH (across all regions) reduced from \$43/MWh and \$3.2/kg H₂ in 2030 down to \$30/MWh and \$2.1/kg H₂ in 2050. Although the LCOE and LCOH were determined by the cost-minimising model in this work, it

is likely that they will become cheaper given optimal location of solar and wind plants (i.e., not necessarily at the iron ore mine); the global weighted average LCOE of new solar PV and onshore wind projects in 2021 were \$48/MWh and \$33/MWh, respectively (IRENA, 2022c).

Green H₂-based steel costs (in 2050, without scrap charging) were accounted to iron ore (28%), solar panels and wind turbines (19%), electrolyzers (9%), production plant (14%), energy storage (6%), labour (9%), other raw materials (e.g. alloys, fluxes) (7%) and operation and maintenance (O&M) (9%). Ore was by far the largest expense item, with greatest variance between region: 20-45% of the total cost. Significant variance in RE infrastructure cost distribution was projected: 3-19% for solar panels, 0-23% for wind turbines and 4-13% electrolyzers. In addition, labour costs were material in differentiating regions; steelworker wages are typically 30% above average (Wood et al., 2020) and H₂, iron and steel production are relatively labour-intensive (refer to Table S3.19). Labour costs constituted 4-21% of total production costs with high wages disadvantaging Australia, Canada, Sweden and the US. If labour costs were excluded, Australia would move up from the 11th to the 3rd lowest-cost producer.

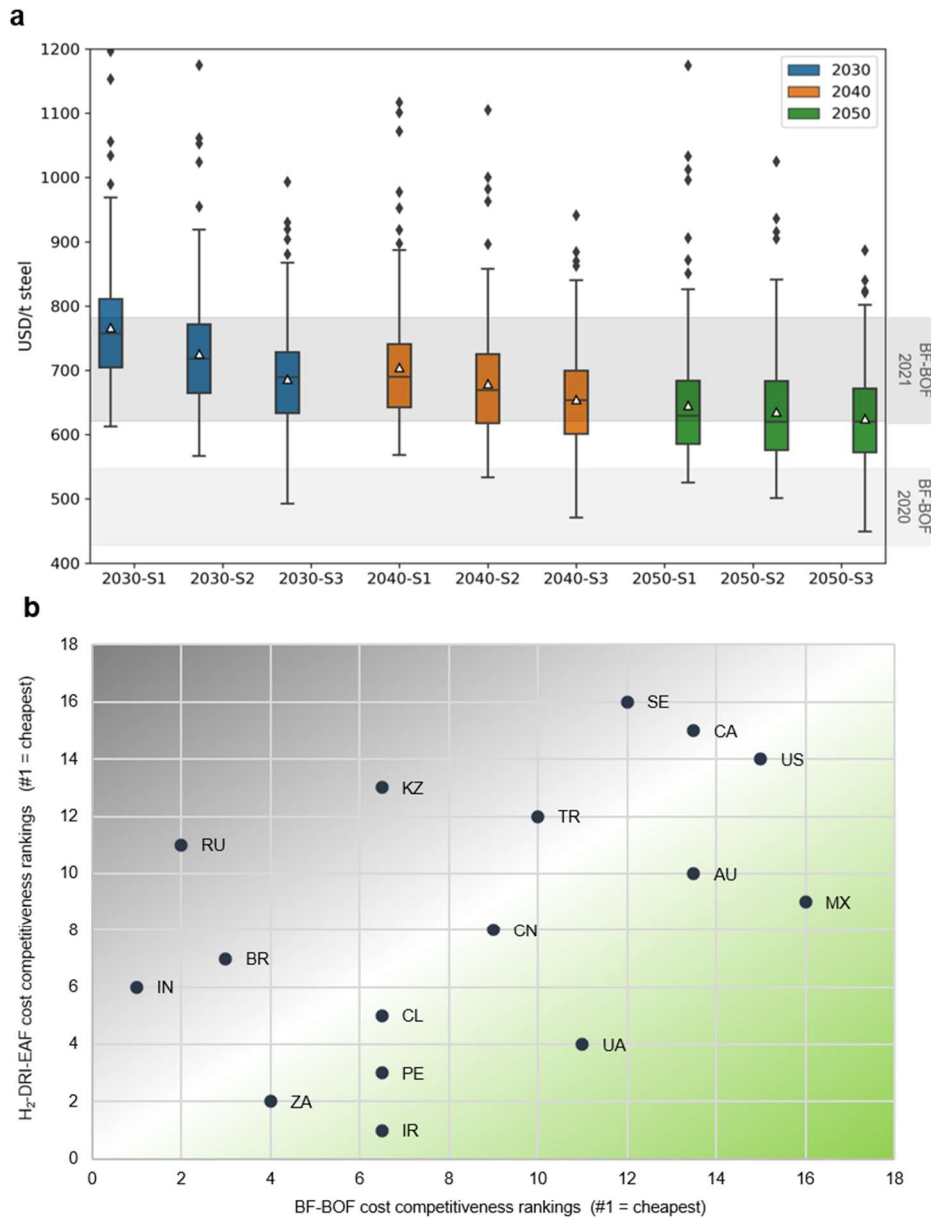


Figure 3.4 Competitiveness of green H₂-based steel with conventional BF-BOF production. (a) Steel production costs, at site (inc. ore) (case S1 = 0% scrap, S2 = 25% scrap, S3 = 50% scrap) compared to BF-BOF costs in 2020 and 2021. For each box and whisker plot, $n = 220$ (44 regions each modelled over 5 historical RE data years), and the mean LCOS ranges from \$766 to \$625. (b) Relative cost competitiveness between BF-BOF (in 2021) and green H₂-DRI-EAF (in 2050) production for all 17 optimised countries, excluding Guinea where steel industry currently doesn't exist. Competitiveness ranking is in descending order from least expensive (#1) to most expensive (#16) steel production. BF-BOF cost data from Transition Zero (2022). The closer the country is placed to the bottom right-hand corner, the more it benefits from the BF-BOF to green H₂-DRI-EAF transition.

Finally, a transition from the conventional BF-BOF production to green H₂-based steel may impact relative regional competitiveness. As illustrated in Figure 3.4b, Mexico and Ukraine may benefit most prominently from the transition, followed by Iran, Australia, and Peru. In contrast, Russia, Kazakhstan, India, Brazil, and Sweden are likely to decrease in relative market competitiveness if H₂-DRI-EAF steel production was established using an islanded solar and wind energy system. However, some of these

countries may alternatively tap into low-carbon and affordable grid-powered electricity (explored in the following section). Countries like Russia may lose their low-cost steelmaking advantage derived from cheap metallurgical coal and natural gas resources, although, competitiveness may be retained through optimising the use of blue H₂ (i.e., H₂ production via steam methane reformation with CCS). Green hydrogen-based steel is likely to shift profitable steelmaking dynamics and open new market opportunities; taking advantage of locally available renewable energy resources is critical to maintaining and growing market share.

3.3.3 Securing cheap, reliable, renewable power for localised production

Affordable, reliable, and wholly renewable electricity is fundamental to competitive near zero-carbon steelmaking. To explore the viability of potential future energy production systems, we compared green H₂-DRI-EAF production using both (variable-load) islanded and (continuous-load) grid energy systems against the conventional BF-BOF production. Unlike the islanded system, energy generation costs of the grid system for 2030 and 2050 are difficult to estimate, therefore the current industrial electricity tariffs were used to indicate the energy cost of the grid system, which vary significantly from \$169/MWh in Brazil to \$41/MWh in Russia, reflecting the current national energy mixes and policies. They were applied in conjunction with projected grid carbon-intensities, which reflect future energy mixes, and carbon taxes, to investigate the required renewables-dominate grid power prices to support a competitive decarbonised steel industry.

By 2050, it was projected that in 7-of-17 studied iron ore-producing countries, at least one of the two green-H₂ based steel production options (i.e. islanded and grid-based) will become competitive with the BF-BOF option, even without the aid of carbon tax. Six countries were projected to produce green-H₂ based steel using the grid-powered system into 2050 as the cheapest option (Guinea, Iran, Kazakhstan, Peru, Russia, and Sweden), however, when carbon prices were accounted for, grid-powered production remained cheaper in just Russia and Guinea. The generally favourable comparison of the variable-load islanded versus continuous-load grid systems stemmed from two aspects. Firstly, although variable-load islanded systems required additional CAPEX to oversize electrolyser and EAF capacities and provide CGH₂ and battery storage, the cost of RE production was favourable compared to grid power prices. In 2050, the average steel production cost savings under the flexible-load islanded system was \$180/t credit for energy, compared to the \$100/t debit for increased capacity of flexible processes and energy/material storage. These relationships would change rapidly given a change in industrial electricity pricing; for grid-powered H₂-DRI-EAF production, 10% change in power price causes a 4% change in LCOS. Secondly, the high projected fossil-fuel shares of many national grids led to significant cost penalties by carbon tax (see Figure 3.5b). Most prominent was Iran's projected reliance on gas-powered electricity meant that even by 2050, the forecast grid emissions intensity was greater than the BF-BOF route at 2.7 t CO₂/t steel (the average for all other countries in 2050 was 0.7 t CO₂/t steel). In countries where the grid is not decarbonising at a swift pace, long-term renewable energy contracts between steel producers and RE providers, or islanded RE systems, will be necessary to produce near zero-emissions steel. In contrast, grid-based systems in Canada and Sweden (closely followed by Brazil) may emit just 0.2 t CO₂/t steel in 2030 (see Figure S3.3b) due to their grid portfolios with

substantial hydropower and nuclear shares. This is already comparable with the islanded system which has emission intensities in the range of 0.1-0.3 t CO₂/t steel across all cases, considering the embodied carbon within solar panels and wind turbines.

The cost competitiveness of the green H₂-DRI-EAF steel production hangs on cheap, CO₂-free power where the variability of renewable resources has been managed. For the islanded system, flexible hydrogen production was far more important than flexible steelmaking to drive down costs; electrolyser oversizing factors ranged from 1.3 to 3.7 (with particularly high oversizing factors for solar-dependent cases, see Table S3.2) whilst EAFs, following continuous DRI production, were oversized far more modestly from 1.1 to 1.4. Whilst we investigated solar and wind resources, other stable and clean electricity sources (i.e. hydropower) are ideally placed for electricity-intensive steel production. For the grid system, operators must concentrate efforts to ensure energy-intensive industries benefit from cheap RE where variability is effectively balanced across time and space. If a renewables-dominate grid could be secured to power H₂-DRI-EAF steel production, an average global electricity price of \$80, \$70 and \$60/MWh (with the lowest being \$62, \$54, and \$46 \$/MWh) would be required in 2030, 2040 and 2050, respectively, to equalise the LCOS (without carbon taxes) across both islanded and grid systems. This is achievable if electricity markets undergo the major anticipated reform in response to growing shares of cheap RE. In 2050, the largest gaps between projected islanded and grid-powered steel costs, and hence between current and target industrial electricity tariffs for competitive grid-powered green H₂-DRI-EAF steelmaking, were observed in Brazil, Chile, and Australia. In these countries, islanded renewable energy systems may be more effective in enabling near zero-emissions manufacturing.

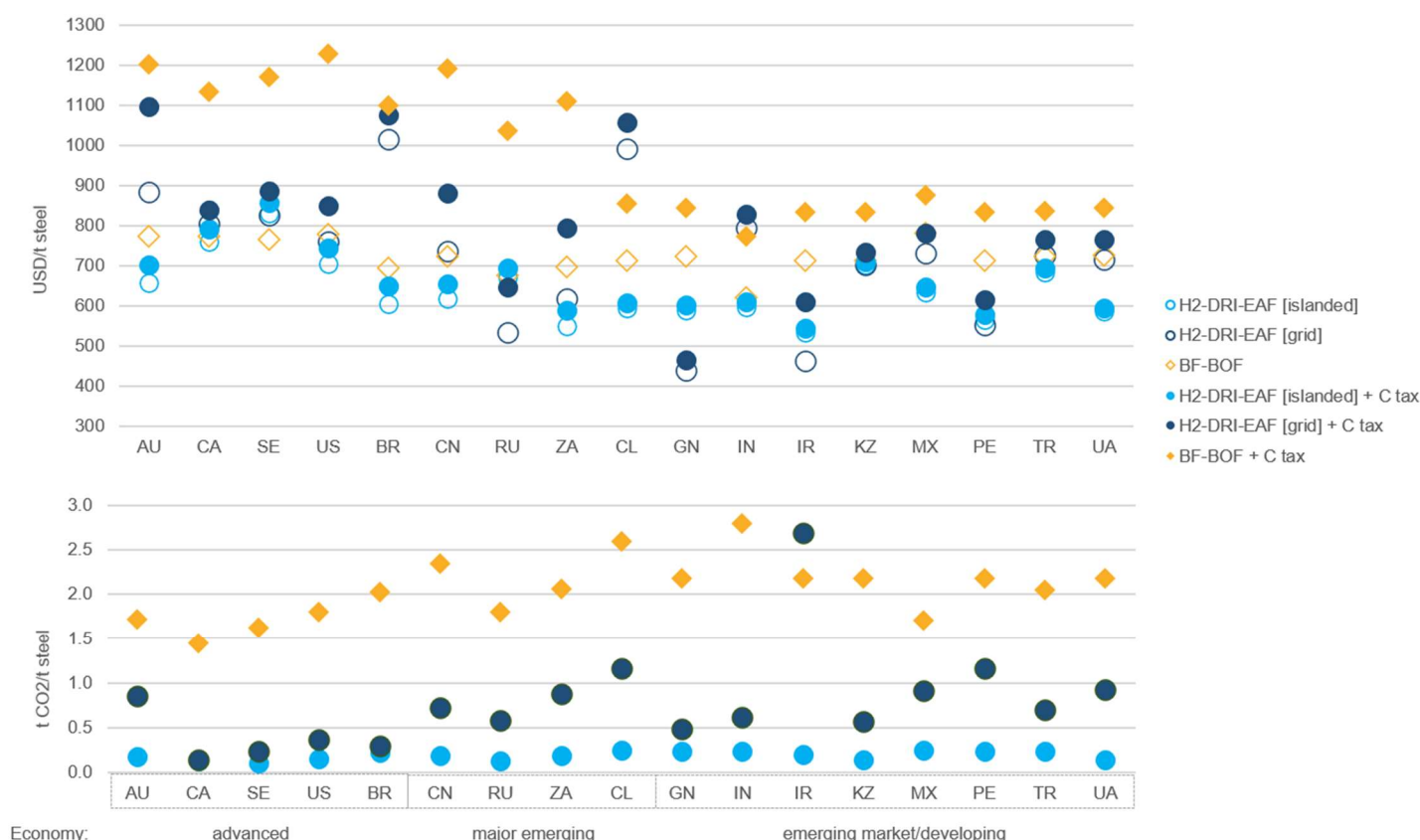


Figure 3.5 Comparison of conventional fossil-based and novel green H₂-based steel production costs and emissions (projects installed in 2050, no scrap charging). (a) Projected LCOS, with and without carbon taxes. (b) CO₂ emission-intensities, where the H₂-DRI-EAF route is modelled with a variable-load islanded energy system, and a continuous-load grid-connected power system. Refer to Figures S3.3 and S3.4 for equivalent graphs for 2030 and 2040 project installation years, respectively.

3.3.4 Global opportunities for green H₂-based steel production

Rapid expansion of LCOS projections from 44 regions to >300 iron ore deposits was achieved using a machine learning model. The ML model was trained using the optimisation results (ML targets) alongside statistical data of solar and onshore wind potential (ML features). ML model accuracy was high, demonstrated by a CoV (R^2) value of 0.96 for predicting the RE cost (\$8/t standard error, 5% of mean) and 0.85 for predicting LCOS (excluding iron ore and labour costs) (\$26/t standard error, 5% of mean) for 1 Mtpa green H₂-DRI-EAF facilities. The cost of solar panels and wind turbines were separated as core cost components requiring further investigation; in 2050, the projected RE costs constituted approximately 20% of optimised LCOS with expected variability (average \$120 +/- \$35/t steel). Both the RE cost and LCOS ML models may be used to aid future supply chain modelling.

The ML models allowed the development of a global picture of green-H₂ based steel potential (see Figure 3.6), revealing that favourable locations were located along the tropic of Capricorn (+23.5°

latitude) and Cancer (-23.5° latitude) where strong solar irradiation is readily accessible. Competitive green H₂-based steel clusters were in Northern and Southern Africa, the central region of South America, Central Asia, and Australia. Interestingly, countries dominating current iron ore production appeared to correlate with competitive green H₂-DRI-EAF steel locations, suggesting that for those regions the green manufacturing opportunity is plausible at scale. A striking opportunity exists in Western Australia, a region offering a stable investment environment, so long as beneficiation can manage the progressive degradation of Pilbara ores.

Additionally, the ML model allowed greater understanding of the influence of RE on green H₂-DRI-EAF steel costs. Multicollinearity analysis of statistical RE data determined the following variables to be selected as features (alongside project installation year) based on their degree of independence: (i) mean hourly solar CF, (ii) CoV of monthly solar CF, (iii) CoV of monthly wind CF and (iv) mean monthly wind CF (see Figure S3.5), where a CoV indicates the degree of variation in the (monthly) data. Feature importance analysis of the LCOS model showed that CoV of monthly solar CF was most important for making predictions, followed by installation year, mean monthly wind CF, CoV of monthly wind CF and median hourly solar CF (very similar results for the RE cost model, see Figure S3.6). Overall, this analysis confirmed the earlier observation from the results of the optimisation model (Section 2.1): low-variability and plentiful solar resources were more important than wind in establishing a cost-effective green H₂-DRI-EAF steel plant, and wind played more a complementary role in RE generation. This may be attributed to the consistent nature of solar resources which are reliably available during daylight hours, as opposed to wind which is more volatile, exhibiting greater daily and seasonal variability.

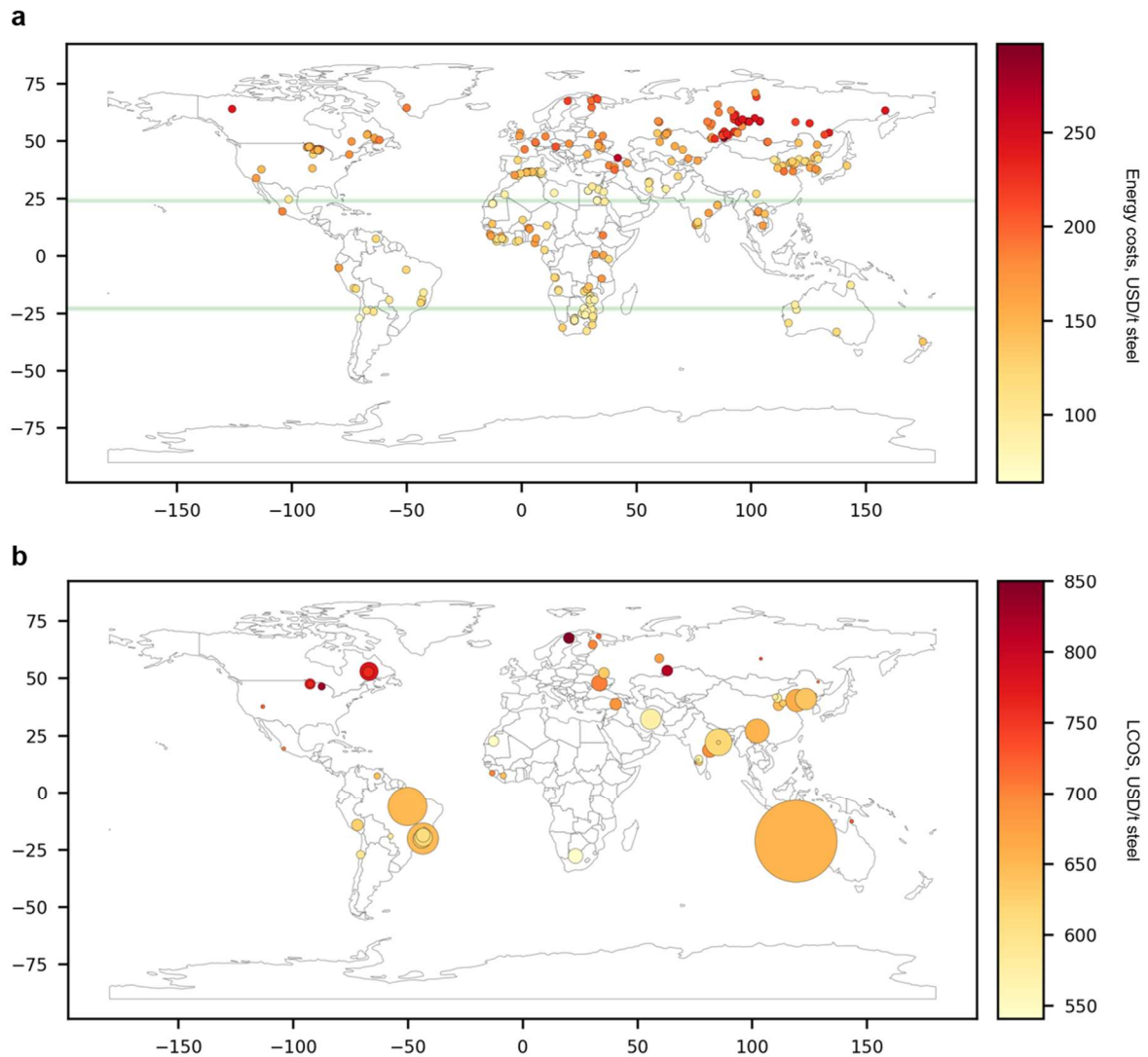


Figure 3.6 Global ML-projected green H₂-DRI-EAF steel costs using islanded solar and/or wind energy systems (projects installed in 2050, no scrap charging). (a) Renewable energy infrastructure costs (i.e. solar panels and wind turbines), for >300 iron ore deposits. (b) LCOS including ore, with markers sized by relative quantity of ore mined on annual basis (mine production data from CRU Group (2022) and U.S. Geological Survey (2022)). Geographical coverage shrinks from 68 to 22 countries which includes all optimised countries, excluding Guinea. LCOS at Kiruna in Sweden was reduced to \$850/t (from \$940/t), which is closer to the optimised LCOS, to control the extreme outlier and enable greater colour graduations over remaining mines (the ML model accuracy was reduced in this extreme northerly location).

3.3.5 Production system feasibility at scale

Up to this point, our global assessments have been made based on steel production facilities with 1 Mtpa capacity, allowing an ‘apples to apples’ cost comparison. However, significant growth in green H₂-DRI-EAF steel manufacturing in certain regions could be hindered by resource constraints and industrial development status. To assess the production system feasibility at scale, national green H₂-DRI-EAF steel industries were sized according to the hypothetical utilisation of extracted ore given the following rates of technology diffusion (i.e., H₂-DRI-EAF steel output of total steelmaking potential): 30% in 2030, 50% in 2040 and 60% in 2050. Using our optimisation modelling results (with 25% scrap charge to EAF), an indicative picture of resource requirements is provided in Table 3.1 for 2050 (with complete

analysis given in Supplementary Data). Land intensity rates of 45 MW/km² and 8 MW/km² for solar panels and onshore wind turbines, respectively, were assumed (National Renewable Energy Laboratory, 2022), alongside a water demand rate of 12 L/kg H₂ for electrolysis (considering 33% losses and 9L/kg stoichiometric minimum) and water recycling rate of 9 L/kg H₂ during DRI. Land availability for RE infrastructure was determined within the regions where iron ore mines exist (rather than the entire country) and constrained by 50% of the available shrubland, herbaceous vegetation and sparse vegetation given by the Copernicus Global Land Cover Map (Buchhorn et al., 2020).

At the assumed level of upscaling, different countries could face a diverse range of resource stresses, such as ore availability, scrap availability, land-intensity (islanded system), grid capacity expansion (grid system) and freshwater demand. While the limitation in the size of ore reserve represents a hard constraint, other stresses could be addressed by measures such as international trade of scrap, significant expansion of power generation capacity, use of alternative low-carbon energy (e.g. nuclear, to reduce land requirement), and use of non-fresh water (and dealing with the additional desalination energy requirement) or implementation of water recycling (to reuse water resulting from iron ore reduction for electrolysis, taking the advantage of co-locating energy and steel production).

In positioning iron ore production as the precursor for green H₂-based steel production, certain countries are confronted with the transition from a raw material export-driven economy to one that is driven by green manufacturing. Australia (and to a reduced extent, Brazil) emerges as a potential future leader in green H₂-based steel manufacturing and exports, given the projection of reasonably competitive green H₂-DRI-EAF production costs and extensive iron ore resources. Fulfilment of vast manufacturing potentials would require significant expansion of renewable energy production. In Australia, this will be most logically supported by islanded energy systems, given that over 4 times the national energy grid capacity would be required in 2050 (assuming 60% technology diffusion), and that iron ore mines are not closely located to established grids. A projected 70-fold increase in Australia's current steel production over the next 3 decades (or even a fraction of this) would need concerted investments and collaboration across private and public sectors, but is far from impossible; the US shale gas industry escalated from near zero output in 2004 to around 2 billion m³ per day in 2020 (U.S. Energy Information Administration, 2022). The greatest challenge facing the country to lock-in favourable economics is to ensure lower-quality ore resources can be directly reduced (e.g. by utilising fluidised bed reactors or additional melting processes to remove impurities) and/or effective ore beneficiation processes are integrated into mainstream mining operations.

Two other countries are also worth mentioning: Sweden, where \$37b of green steel investment has already been directed (Vogl et al., 2021c) has very high quality ore reserves but of modest magnitudes, which will limit the scope for producing green H₂-based steel from local ore. Also in China, which is currently dominating global steel production (53%) to primarily serve their extensive domestic markets, 90% of its steel production is currently primary (ore-based) production (worldsteel, 2022). In the transition to green H₂ based steel production, increasing the mix of scrap in the feed to EAF would be beneficial to capitalise on the immense volumes of steel scrap available.

Table 3.1 Feasibility considerations for green H₂-DRI-EAF production using islanded RE systems, at scale. Analysis is based on forecasted steel output, determined to be a function of current ore output. Data shown for 2050 production system which assumes utilisation of 60% of national produced iron ore and 25% scrap charge to EAF (refer to Supplementary Data for complete analysis). Negative values in the “scrap surplus” column indicate deficits.

Country	Ore production, 2020	Hypothetical H ₂ -DRI-EAF steel production	Gross iron in reserves	Iron ore reserve life remaining	Steel production expansion factor (by output)	Scrap surplus	Land consumption of RE infrastructure	Ratio of RE land demand to regional availability	Net water demand	Net water demand as factor of current industrial withdrawal	Energy demand	Ratio of energy demand to current national consumption
	Mtpa	Mtpa	Mt	years	-	Mtpa	1000 km ²	-	10 ⁹ m ³ /yr		TWh/yr	-
Australia	912	395	25000	44	71.05	-113	41.78	0.04	76	27.76	1122	4.19
Brazil	388	173	15000	61	5.07	-32	15.43	0.05	38	3.64	491	0.75
Canada	60	25	2300	64	1.98	-2	5.18	0.03	5	0.18	72	0.11
Chile	16	7	-	n/a	5.85	-1	0.33	0.01	2	1.10	20	0.22
China	360	157	6900	31	0.16	431	20.49	0.17	32	n/a	447	0.05
Guinea	60	28	-	n/a	0.00	-8	2.05	0.72	7	110.79	79	0.85
India	204	89	3400	27	0.82	83	7.96	0.62	21	1.21	252	0.15
Iran	50	23	1500	46	0.88	-7	1.53	0.02	5	4.71	65	0.18
Kazakhstan	63	9	900	71	2.09	-3	1.34	0.02	2	0.29	25	0.22
Mexico	15	7	-	n/a	0.35	11	0.57	0.16	2	0.18	19	0.06
Peru	13	6	1500	169	5.53	2	0.36	0.04	1	0.43	18	0.31
Russia	100	49	14000	201	0.67	14	11.51	1.93	9	0.32	138	0.12
South Africa	56	25	670	19	4.47	15	2.12	0.01	5	1.27	70	0.29
Sweden	36	18	600	24	3.80	-2	5.05	0.30	4	2.62	51	0.30
Turkey	15	6	38	4	0.16	23	0.81	0.33	1	1.35	17	0.05
Ukraine	79	34	2300	47	1.64	-8	5.34	1.88	7	1.55	98	0.63
United States	38	17	1000	41	0.20	83	2.37	0.22	3	0.02	48	0.01

In addition to the resource requirements discussed above, other considerations for the successful transition to green H₂-based steel include: (i) reskilling and redistributing steelworkers, (ii) land competition between renewable energy infrastructure, agriculture, and CO₂ sequestration (Harvey & Pilgrim, 2011), and (iii) supply chain bottlenecks including rare earth mineral supply for solar panels, electrolyzers and batteries (Grandell et al., 2016). These factors deserve careful treatments in future business and policy decisions.

3.4 Discussion

The favourable locations identified in this work for co-locating the production of iron ore, RE and steelmaking, represent areas where such a simple supply chain is likely to make economic sense. For such cases, product shipping costs still need to be added to the overall costs. Fortunately, ideal locations for green H₂-DRI-EAF facilities were within reasonable distance to the coast and its ports. Added costs for FOB and CFR (to Qingdao, China) were minimal: global average of 3% added cost burden for inland transport and 7% for marine transportation (refer to Table S3.3). It is unlikely that transport of product will dictate production facility locations, but proximity and regional free trade

agreements will support strategic investments. On the other hand, the trade and transport of primary or intermediary products (iron ore, green H₂ or HBI) should be explored. Depending on the relative location of high-quality iron ore, renewable energy, and demand markets, steelmaking facilities may not necessarily need to be placed in locations optimal for production efficiency, but rather a favourable location close to critical supply chain links.

In this work, the optimised LCOS using the islanded production system was primarily affected by the regional quality of RE and iron ore, the year of installation and the fraction of scrap. A comparison with literature, where projected LCOS of H₂-DRI-EAF steel has been estimated at \$778 (Vogl et al., 2018), suggests that differences in cost projections are present due to different assumptions with respect to the RE and steel production system and costing basis. Here, we discuss multiple factors particularly important for the costing undertaken in this study.

- **Iron ore quality at mine-level.** Whilst spatial resolution of renewable energy data was at coordinate-level, the best available ore quality data was at national-level, limiting the accuracy of beneficiated ore costs. In addition, characterisation of ore deposits according to composition (hematite, magnetite, goethite, limonite, etc.) was scarce, and consequently the assumption made that all ore reserves were hematite (the most common iron ore type). Given better data, we would have performed differential beneficiation and reduction analysis to determine more accurate production costs. The simplified linear cost equations for DR-grade ore applied in this study are illustrative of the added cost burden of beneficiation, but not conclusive.
- **RE potential.** The nature of optimisation modelling using historical RE data caused the assumption of planned flexibility, which is impractical. Inter-annual variability was addressed in this work by running the optimisation models repeatedly with different historic annual RE profiles across five years (2015-2019); the difference in LCOS projections between repeated runs appear to be modest across most locations (see error bars in Figure 3.3b). Nevertheless, modelling over a longer period, e.g., 20 years of historical RE data could yield results that can be compared with those from this work to further increase confidence. Furthermore, this global study considered solar and (onshore) wind as RE sources for the islanded system; further detailed regional studies could explore other renewable energy resource integration, namely offshore wind, hydropower, and biomass.
- **Industrial electricity tariffs.** For assessing grid-based systems, we used current industrial power prices (of 2018), in absence of clear projections of future power prices, to reflect on the energy system conditions for competitive steelmaking, and hence required electricity market reform. These tariffs are highly unlikely to stay constant due to changes in energy portfolios, commodity prices (namely natural gas and coal), network costs (likely enhanced distribution infrastructure due to integrated RE systems), need for RE storage, and taxes/levies. National grids must deal with transitional challenges including RE supply scarcity aligning with peak demand. Steelmaking facilities may be able to take advantage of dynamic pricing, where

production is aligned with demand troughs, or establish long-term renewable energy contracts with energy providers to receive stable, low-cost renewable electricity.

- **Flexibility in green H₂-based steel production.** This work considered flexible operation of the electrolyser and the EAF. Other means of flexibility left unexplored include altering the load factor of the DRI shaft furnace (e.g., 70-100%) and allowing a flexible scrap charge for every batch (scrap fraction becomes an annual rather than hourly constraint, allowing the hourly level to vary). Ideally, scrap charge to the EAF should be set based on regional scrap flows, including import and export. Whilst we explore islanded and grid-powered energy systems separately, semi-islanded energy systems with varying degrees of dispatchable power may lead to cost reductions.

Finally, several further challenges of H₂-DRI-EAF steel making require attention. In this work, we have considered the beneficiation requirements to uplift the quality of the currently available ore to DR-grade. Considering that DR-grade ore constitutes just 4% of current global seaborne trade, and accessible high-grade ore reserves are decreasing with cumulative extraction (Nicholas & Basirat, 2022a), scale-up of iron ore beneficiation competence and capacity is a global priority. Especially in Australian Pilbara ores (responsible for 37% of annual global iron ore output (U.S. Geological Survey, 2022)), the increasing presence of goethite (an iron oxyhydroxide) in extracted ore is a concern due to its high porosity and friable texture, leading to ultrafines generation (Vining, 2017). Whilst ultrafines improve sinter production efficiency, they must be avoided in DR shaft furnace operation due to the counterflow reduction mechanism. Iron ore producers are aware of the threat of increasing DR production to their product marketability; ore reserves suitable to serve the DR-grade market remain limited (Nicholas & Basirat, 2022b).

If the raw material challenge cannot be met by supply, downstream processing must become more flexible. Two flexible processing options have emerged: (i) BF-grade iron ore pellets may be used in the DR shaft furnace, however, with an additional process pre-EAF to melt the sponge iron and remove impurities via slag formation (DRI-melter-EAF), and (ii) the use of DR-grade (or potentially BF-grade) iron ore fines in DR with fluidised bed reactors, so long as the fluidisation velocity is maintained above the minimum and the agglomeration phenomenon of 'sticking' (increased adhesion and friction among particles) is controlled (Nicholas & Basirat, 2022b; Wolfinger et al., 2022a). Nevertheless, both supply- and demand-side innovations are required to enable productive green H₂-based DRI-EAF supply chains.

In addition to the critical issues around iron ore supply, several other challenges have been identified for the green H₂-DRI-EAF route, most notably the maintenance of metallisation degree in the shaft furnace in light of the resistance of diffusion of H₂, and the different melting characteristics of carbon-lean H₂-DRI in the EAF (Kim & Sohn, 2022). Despite the current success of H₂-DRI-EAF with pilot-scale testing as demonstrated in HYBRIT (SSAB, 2022), further technical developments are still required to fully resolve these issues.

3.5 Conclusions

This study benchmarked green hydrogen-based steel market competitiveness for 17 of the most important iron ore producing countries and projected for over 300 global locations through combined use of optimisation modelling and machine learning. Competitive renewables-based steel production was shown to be located nearby the tropic of Capricorn and Cancer, characterised by superior solar with supplementary onshore wind, in addition to high-quality iron ore and/or low steelworker wages. Large-scale implementation requires attention to the abundance of suitable iron ore and other resources such as land and water, technical challenges associated with direct reduction, and future supply chain configuration. Australia and Brazil advantageously possess both high-quality renewables and large quantities of iron ore deposits; given iron ore quality constraints can be overcome (likely through enhanced ore beneficiation or additional smelting processes) and Australia's wage growth can be controlled, these nations are well-positioned to invest widely in a green iron and/or green steel export industry. If coking coal prices remain high, green H₂-based steel could attain competitiveness in favourable locations from 2030 and further improving towards 2050, using variable-load islanded energy systems. In comparison to sourcing electricity from the grid, islanded renewable energy generation using solar and wind appeared generally more preferable, except in regions with high renewable energy shares in the grid portfolio and competitive industrial electricity tariffs. Electricity market reform and expansion to enable affordable and abundant renewable energy supply to electricity-intensive sectors, or competitive long-term renewable energy contracts established directly between steel manufacturers and renewable power plants, would be required to justify selection of grid-power rather than captive power plants in most locations. Furthermore, the co-location of electrolysis, iron ore reduction and electric steelmaking could be an effective supply chain configuration, but more importantly this global analysis provides a foundational building block from which to explore more complex supply chain networks.

Chapter 4. Regional Green Hydrogen-Based Steel Supply Chains

Overview

This chapter presents the following published article: Devlin, A., & Yang, A. (2022). Regional supply chains for decarbonising steel: Energy efficiency and green premium mitigation. *Energy Conversion and Management*, 254, 115268. <https://doi.org/10.1016/j.enconman.2022.115268>. The published article presents monetary terms in AUD, but here has been converted to USD. The corresponding Supplementary Information is contained within Appendix II.

Among all authors who contributed to the research, A.D. conceptualised the study, developed the model, analysed the results, and wrote the manuscript, A.Y. supported with the conceptualisation, provided feedback on the modelling, and revised the manuscript.

This second piece of original work explored the geography of resources through strategic trade links to provide insights into how supply chains may be reconfigured to support renewables-based steel production. This builds on the first research project which identified Australia's potential to benefit from the green steel transition, exploring its prospective role as a green product manufacturer, rather than raw materials producer, in the Asia-Pacific region. Too, the supply chain assessment advances from co-location to dislocation of hydrogen, iron, and steel production. Focusing on the energetic and techno-economic assessment of potential green steel supply chains, this study investigated the H₂-DRI-EAF production route enabled by renewable energy and deployed in regional settings. New trade paradigms are introduced involving H₂ and HBI transportation, supporting the decoupling of iron and steel production. The hypothesis was tested: co-locating manufacturing processes with renewable energy resources will deliver the highest energy efficiency and lowest costs. Australia, the world's largest iron ore producer with ample land and significant proven solar and wind resources, was paired with nearby Japan, the world's second largest steel producer with a clear lack of available land resources and renewables deficit. Too, the Australia-Japan relationship is mature, collaborative, and integral to the strategic and economic interests of both countries, providing an ideal case study to investigate green iron and steel trade under the framework of supply chain redistribution and regional resource pairing in a decarbonised future.

4.1 Introduction

The globalised trade of steel means that the geography of resources and the decarbonisation of the sector are closely linked. Supply chain relocation associated with the steel production paradigm shift to

net zero is an emerging area of research. Of particular interest is the binational partnership between Australia, a mineral and energy exporter, and Japan, a steel producer and exporter. Relevant trade links are already established between the two nations; Japan's imports of Australian iron ore represent 4% of global ore trade (8% Japanese share of Australia's exports which is 53% of global trade) (DISER, 2020b). Japan is the second largest global steel exporter after China (worldsteel, 2020a), serving Asia's developing economies. Moreover, both nations are actively promoting a hydrogen-based economy and collaborating on the Hydrogen Energy Supply Chain Project, an initiative which aims to produce and transport blue hydrogen from Latrobe Valley, Australia, to Kobe, Japan (COAG Energy Council, 2019). Hence, the Australia-Japan partnership was selected as a case study for global clean energy-driven manufacturing.

This study attempts to evaluate how different supply chain configurations affect the technical and economic performance of a regional green steel initiative. More specifically, this work tests the hypothesis that co-locating high-quality renewable energy resources, iron ore reserves, and manufacturing facilities will drive energy and cost efficiency through a comprehensive energetic and techno-economic assessment of the Australia-Japan link for green steel. Zero carbon H₂-DRI-EAF supply chain configurations are established for representative time periods (i.e., 2030 and 2050) and vary in the spatial locations of DRI and EAF, each encompassing renewable energy supply, iron and steel production and shipping. While the assessed options are similar to the "pathways" considered by Wood et al. (2020), they are investigated here with detailed modelling of the processes of energy production and storage, steel production, and transport, to derive energy efficiency and costs, which is necessary for enabling comprehensive and transparent comparisons between different options. Furthermore, the assessment has considered two different H₂ energy vectors (LH₂ and NH₃); to the authors' knowledge, this is the first comparative study of the two energy vectors within the context of complete green steel supply chain. Such understanding is important for revealing key factors affecting the performance at the entire supply chain level, hence providing valuable guidance to future decision making in technical, business and policy development.

This work aims to reveal how different designs of the Australia-Japan regional link affect (1) the overall energy efficiency, and (2) the economic competitiveness of fossil-free steel in light of the acknowledgement of the financial burden of the technological solution as a major challenge of steel decarbonisation (Fan & Friedmann, 2021). Quantification of green premiums (the additional cost of fossil-free alternatives) enables establishment of baseline market competitiveness, and determination of carbon prices which have been proven influential in incentivising industrial emitters to enhance energy efficiency and invest in renewables (Wong & Zhang, 2021). The correlation between manufacturing efficiency, economic competitiveness, and carbon emission reductions has been investigated in the Australian context (Foumani & Smith-Miles, 2019), which this study utilises the principles of. The adoption of a systems perspective and binational case study is intended to deliver results relevant to industrial change on a global stage.

4.2 Methods

In this section, the system definition and cases covered by this study are first introduced, followed by a technical description of the four major decarbonised steel production capabilities: (i) renewable energy supply, (ii) iron and steel production, (iii) H₂ production, storage, and conversion, and (iv) shipping. Approaches to energy and economic assessments are also established. For each case, the energy assessment quantifies total energy consumption per tonne of steel product and derives pathway energy efficiency (from renewable energy supply to end use) of key subsystems. On the economic side, LCOS is the key metric quantified, complemented by the LCOE and LCOH as the core constituents of the fossil-free production system. In general, these assessments have drawn on literature data (such as energy efficiencies and technology costs) where reliable sources are available, which are supplemented by results of process simulation carried out in this work for less-studied subsystems (such as DRI and NH₃ cracking).

4.2.1 System definition and cases for analysis

The prerequisites for green hydrogen-based steelmaking are abundant renewable energy, iron ore and water, which makes the Pilbara region of Western Australia a prime location. The fossil-free supply chain system following the H₂-DRI-EAF technical route was modelled to produce 40 million tonnes of semi-finished steel (SFS) per year, based on current Australia-Japan iron ore trade, with both the iron ore and all the required energy sourced from the Pilbara region in Western Australia. The objective was to assess (and minimise) the system's energy consumption and price premiums – the difference between one tonne of fossil-based steel and one tonne of hydrogen-based steel.

Twelve unique cases were studied with three key variables: supply chain (SC) design, energy vector and shipping fuel (LH₂ or NH₃), and year (2030 or 2050), as detailed in Table 4.1. Alike Wood et al. (2020), multiple energy and material trade alternatives were investigated, which consequently differed in the location of DRI, EAF and supporting production processes. SC1 followed the “traditional” route of Australia exporting energy and iron ore for iron and steel production in Japan, differing from present-day practice by substituting coal with hydrogen. SC2 exported HBI, the intermediary product between DRI (iron production) and EAF (steel production), along with hydrogen to complete steel production in Japan. Although DRI is an exportable commodity, it is prone to oxidation; in comparison, HBI removes the challenge of sealing the cargo in an inert gas atmosphere (HBI Association, 2009). SC3 exported semi-finished steel to Japan, completing all iron and steel production processes in Australia. Under all cases, the premise is that either direct renewable energy, or hydrogen produced via renewable energy, must be utilised to energise the entire supply chain. Hence, hydrogen exports serve both energy and ore reductant requirements in Japan. The prospect of Japanese production of renewable energy was not considered as Japan is a small and densely populated nation with minimal land available for the installation of solar PV panels and wind turbines, and whilst offshore wind generation is possible, it is expected to cost 50% more per MWh than onshore solar PV (Cheng et al., 2022).

The consideration of the two alternative energy vectors, LH₂ and NH₃, both among potential H₂ carriers for long-distance transport, was to allow a comparison between the two options within the context of a

regional supply chain for decarbonised steel. In terms of the timelines, 2050 was selected to align with net-zero carbon targets under the Paris Agreement, with 2030 as a medium-term milestone for emission reductions.

The three supply chains are illustrated in Figure 4.1, distinguished by processes during four discrete stages: Australian production, export preparation, marine transportation, and Japan production. For simplification, intermediary energy storage and conversion processes including CGH₂ storage, fuel cell power generation and combustion for heat generation, are not shown. For all cases, the shipping route was from Port Hedland, Australia, to Port Osaka, Japan, quantified at 3497 nautical miles (equal to 6476 km; S&P Global Platts (2021)).

Table 4.1 Variables applied within the twelve unique cases for the binational supply chain analysis, and notation for each.

		Time period	2030		2050	
		Energy vector and shipping fuel	LH ₂	NH ₃	LH ₂	NH ₃
Supply chain design	SC1	Export H₂ and iron ore for H ₂ -DRI-EAF iron and steel production in Japan	SC1-LH ₂ -2030	SC1-NH ₃ -2030	SC1-LH ₂ -2050	SC1-NH ₃ -2050
	SC2	Export H₂ and HBI for EAF steel production in Japan	SC2-LH ₂ -2030	SC2-NH ₃ -2030	SC2-LH ₂ -2050	SC2-NH ₃ -2050
	SC3	Export of decarbonised steel to Japan as semi-finished products (LH ₂ /NH ₃ only required for shipping fuel)	SC3-LH ₂ -2030	SC3-NH ₃ -2030	SC3-LH ₂ -2050	SC3-NH ₃ -2050

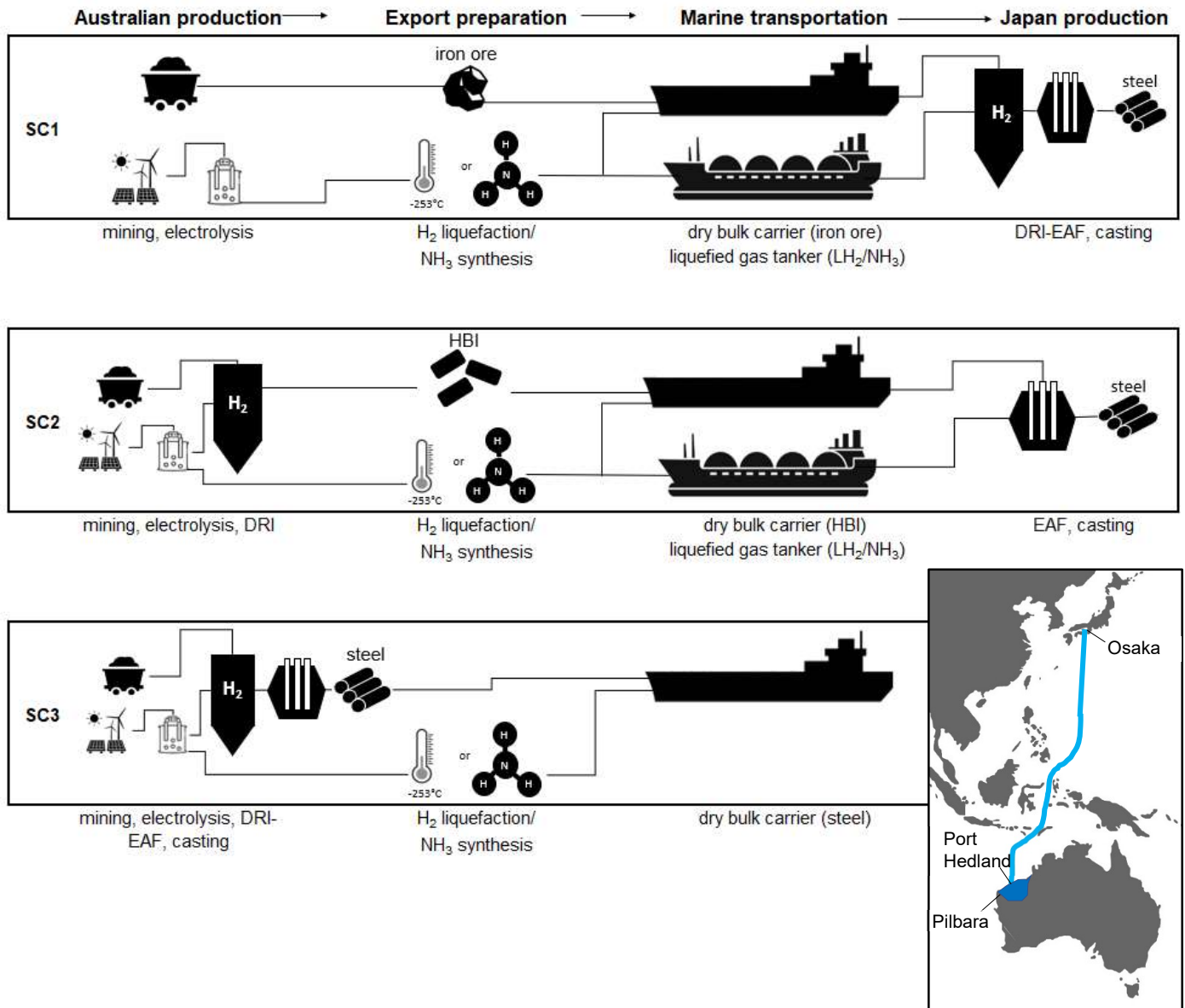


Figure 4.1 Simplified supply chain illustrations for the binational analysis which indicate the location of major production processes and mass and/or energy export products. A map of the shipping route from the Pilbara region of Western Australia to Osaka in Japan is also shown.

Across all the supply chain configurations, hydrogen (or NH_3 as an alternative form) has four critical end-use applications:

- (1) **Feedstock**, to reduce iron ore to sponge iron in the shaft furnace.
- (2) **Heat for production**, to provide thermal energy (converted via combustion) for production processes.
- (3) **Power for production**, to provide electrical energy (converted via fuel cells) for production processes.

- (4) Transport**, to provide electrical energy (converted via fuel cells) to power electric motors which propel shipping vessels.

Besides this, hydrogen serves two critical energy storage roles: in the form of LH_2/NH_3 for long-distance transportation from Australia to Japan (as introduced above) and in the form of CGH_2 to provide a buffer between those processes to operate in Australia with a constant load and the VRE supply.

This work did not consider domestic transportation (and any associated intermediate storage) and loading/unloading at ports, which were deemed negligible compared to the major components of the system. Embodied emissions of related infrastructure have also been excluded.

4.2.2 Technical description and energy assessment

Here, the key characteristics of all the system components and the approaches adopted for energy assessment are presented. Further equations and parameters for energy modelling are detailed in the Supplementary Methods (of Appendix II).

4.2.2.1 Energy demand and renewable energy supply

Whilst variable renewable energy matching is ideal (e.g., sunny in the day, windy at night), it is often unachievable and battery storage is needed to manage these troughs. The 100% VRE systems were modelled in Homer Pro microgrid software which optimised for lowest NPV. Despite allowing for both solar and wind energy assets in the optimisation, all cases opted for a design with zero reliance on wind power. Whilst counterintuitive, this reflected the high costs of wind turbines compared to solar panels, and the high variability of wind velocities. The diurnal solar cycle necessitated short-term (daily) energy storage to deliver constant power and/or H_2 demands of inflexible processes operating in the Pilbara. Such processes included DRI (and the associated H_2 heating and compression), EAF and NH_3 synthesis. In contrast, flexible processes including electrolysis and H_2 liquefaction were considered to fully accomplish their daily load during the daylight hours and therefore did not require the aid of energy storage. Since a hydrogen buffer (to supply DRI and NH_3 synthesis) was an important part of the required storage capacity, CGH_2 (as opposed to other options such as batteries) was chosen for implementing the short-term energy storage. To provide a quantification of the diurnal distribution of energy demands by the flexible and inflexible processes, the 24-hour duration was divided into a daylight period (denoted by VRE_{on}) and a non-daylight period (denoted by VRE_{off}), with the length of the former set to 9 hours which represents a conservative estimate as daylight hours in Pilbara are typically 10-12 hours/day.

The daily demand for all flexible processes was met only during VRE_{on} , in unison with the dynamic VRE supply. An inflexible process, on the other hand, required constant energy and/or hydrogen feeds during both VRE_{on} and VRE_{off} with the latter period supplied by the CGH_2 storage. The total demand during the VRE_{on} period thus comprised both the demands of the flexible processes and that of operating CGH_2 . Note that the consideration of flexibility concerns only the energy supply to the processes that occur on the Australian side of the supply chain; the processes to take place in Japan were always supplied by the energy shipped from Australia in either form of H_2 carrier (LH_2 or NH_3). To further illustrate the energy routing in the system, Figure 4.2 shows three distinct energy pathways for one of the energy

demands, H₂ as DRI reductant, depending on the process location and energy vector. Energy pathways for all end-use applications are detailed in Table S4.1.

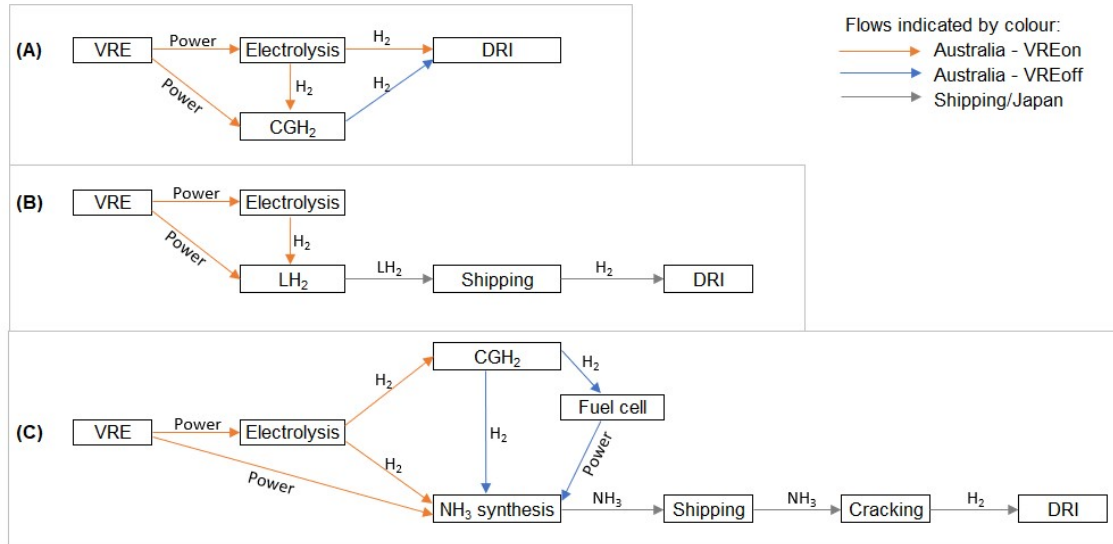


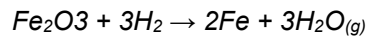
Figure 4.2 Energy pathways for H₂ serving DRI as reductant. When DRI occurs in: (a) Australia, (b) Japan with LH₂ as the energy vector, and (c) Japan with NH₃ as the energy vector.

It is worth emphasising that the two time periods (VRE_{on}, VRE_{off}) were defined solely for the purpose of composing the diurnal electricity demand profile for each case. The demand profile defined as such formed input to Homer Pro where the actual, location-specific (typical) diurnal variation of the available renewable energy was used to compute the cost-optimal design of the renewable energy system that can satisfy the specified demand profile/.

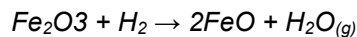
4.2.2.2 Iron and steel production

Iron ore, 95% hematite (Fe₂O₃) and 5% inert material by mass, is reduced by hydrogen in the shaft furnace, as shown in Equations 4.1-4.2:

Equation 4.1 Hematite reduction by hydrogen into elemental iron and water



Equation 4.2 Hematite reduction by hydrogen into iron oxide and water



The shaft furnace operates at 900°C and atmospheric pressure, and the metallisation rate is taken as 94%. Before entering the furnace, H₂ is heated to 900°C and compressed from 1 bar to 2 bar, to overcome the pressure drop in the shaft furnace. Using Aspen Plus Modelling (see Supplementary Methods), the energy consumption was calculated to be 0.45 MWh/t liquid steel (LS) for H₂ heating pre-DRI and 0.065 MWh/t LS for H₂ compression pre-DRI. The outputted sponge iron was either fed directly to the EAF or briquetted to produce HBI for export.

EAF power consumption was determined based on literature data, 2.4 MJ/kg LS (Krüger et al., 2020), adjusted according to the chosen metallisation rate. Scrap, carbon, and lime additions were not considered in the EAF process. A continuous caster followed the EAF where blooms, billets and slabs were formed, the semi-finished state for further processing (not considered in this work). Casting energy demand was taken from literature data, 0.0103 MWh/t LS (IEAGHG, 2013). Overall, the following key material flow data were derived: 1.5 t ore/t steel, 1.1 t HBI/t steel and 52 kg H₂/t steel (note that hereafter, “steel” refers to “semi-finished steel”). Since these processes are either commercial or modelled with a theoretically rather optimal design in the case of DRI, none was considered to incur an efficiency improvement from 2030 to 2050.

Energy supply to these processes depended on their location and the timing. Thermal energy was either produced using electrical heating during VRE_{on} in Australia (with efficiency of 90%), or via H₂ (with H₂ from intermediate CGH₂ storage during VRE_{off} in Australia, or with LH₂ in Japan) or NH₃ (in Japan) combustion (with efficiency of 85% based on the lower heating value (LHV) of the fuel). Power was either directly served as VRE (during VRE_{on} in Australia) or indirectly through fuel cells fed with H₂ from intermediate CGH₂ storage (during VRE_{off} in Australia) or LH₂/NH₃ exports (in Japan). For energy carrier-to-power conversion, solid oxide fuel cell (SOFC) technology was used as an advantageous high-temperature operation suitable for stationary, large-scale power generation (Mekhilef et al., 2012). Additionally, SOFCs support the direct use of both H₂ and NH₃, avoiding the additional NH₃ cracking process (McKinlay et al., 2020). Stationary SOFC efficiency value of 60% (based on LHV) was used for 2030 (Peters et al., 2016; Scataglini et al., 2015) with modest increase to 64% in 2050.

4.2.2.3 H₂ production, storage, and conversion

Carbon-free hydrogen is produced via electrolysis of water using renewable energy. The alkaline electrolyser, chosen in the modelling, operates at a temperature of 70°C and atmospheric pressure with efficiency of 68% in 2030 and 75% in 2050 (IEA, 2019). The electrolyser design capacity of 86.5% is taken from industry data (Thyssenkrupp, 2018). Based on a large-scale electrolyser size of 100 MW, 2.04 t H₂/hr and 2.25t H₂/hr is achievable per module in 2030 and 2050, respectively.

Aboveground CGH₂ in steel tanks at 150 bar (and 25°C) was selected for short-term storage due to its rapid ramp-up/down and high cycle lifetime (Gallo et al., 2016), and uncertainty avoidance from alternative geological storage based on salt deposits or depleted gas reservoirs (Geoscience Australia, 2021). Steel is a common material for compressed gaseous hydrogen storage up to 250 bar (Hadjipaschalis et al., 2009). Using Aspen Plus, compression energy demand was determined as 2.68 kWh/kg H₂ which is in alignment with literature (IRENA, 2020).

Liquefaction of hydrogen gas (LH₂) requires intensive energy to reach temperatures less than -253°C at a pressure of 1 bar. Commercial hydrogen liquefaction plants consume 30% of hydrogen's dispensable energy at 10kWh/kg H₂ (Berstad et al., 2021). Future reductions for large-scale plants to 6kWh/kg H₂ have been forecasted for larger plants with process improvements (Aasadnia & Mehrpooya, 2018; Berstad et al., 2021; Stolzenburg et al., 2013). These two energy intensity levels were adopted for 2030 and 2050, respectively.

NH₃ synthesis energy demand, to drive the air separation and Haber-Bosch processes, was taken from literature as 0.7 kWh/kg NH₃ (Nayak-Luke et al., 2018). NH₃ cracking was required pre-DRI (SC1) as pure H₂ was necessary in the shaft furnace. The use of NH₃ as the direct reductant of iron ore (Hosokai et al., 2011) is potential, however rarely examined in literature and not applied in this model. Using Aspen Plus and a similar approach to (Giddey et al., 2017), the cracking energy was modelled using an NH₃ conversion rate of 95%, H₂ recovery rate of 85% and heat recovery efficiency of 85%. Thermal energy consumption rate was determined to be 0.072 MWh/t NH₃, supplied by NH₃ combustion with overall cracker efficiency of 79%.

4.2.2.4 Shipping

Dry bulk carriers were used to transport iron ore, HBI and steel. Iron ore is a 'major bulk' commodity, generally shipped in capesize vessels (>100,000dwt) as a minimum. Australia's iron ore producers are capped by berthing capacities at Port Hedland (Pilbara Ports Authority, 2020) and currently use Newcastlemax vessels (BHP, 2020). The largest vessel that HBI is transported in is the panamax (65,000–99,999dwt) (Hot Briquetted Iron Association, 2009), and the same has been assumed for steel as a comparable 'minor bulk' commodity (UNCTAD, 2020).

A 160,000m³ liquefied gas tanker was used to transport LH₂ at -253°C and LNH₃ at -33°C within low-vacuum insulated spherical tanks (Al-Breiki & Bicer, 2020b). Boil-off gas (BOG) was estimated at 0.2%/day for LH₂ (Wijayanta et al., 2019) and 0.02%/day for NH₃ (Al-Breiki & Bicer, 2020b).

Shipping, a hard-to-electrify mobility sector, can utilise electrofuels with internal combustion engines (ICEs) or fuel cells (FCs) for propulsion power. Whilst development of large-scale electro-fuelled ICE systems may precede fuel cells with electric motors by 5-10 years (due to technology maturity of ignition engines) the higher-efficiency fuel cell technology will likely prove more economical in the long-term with the added benefit of no dangerous nitrogen oxide emissions (Ash & Scarbrough, 2019). Both LH₂ and NH₃ were investigated as marine shipping fuels and adopted the mobile FC with electric motor propulsion system.

The proton exchange membrane fuel cell (PEMFC) is the most mature H₂-powered fuel cell technology, advantaged by a low operating temperature, small module size and decreased costs. PEMFC operation is moderately efficient at 50-60%, however heat recovery is unfeasible and pure H₂ is required. This technology has been ranked first for marine applications across a broad range of criteria by the European Maritime Safety Agency (Tronstad et al., 2017). For NH₃ fuel, the SOFC is more appropriate as pure H₂ inputs are not required, removing the need for NH₃ cracking. SOFC operates at high temperatures and can reach an efficiency of 85% with heat recovery, or 60% without (Tronstad et al., 2017). Hence, H₂-PEMFC and NH₃-SOFC were chosen for modelling. In the absence of energy efficiency targets specifically for marine shipping applications of FCs, the U.S. Department of Energy targets for long-haul trucks were utilised; 68% in 2030 and 72% in 2050 (Marcinkoski et al., 2019).

To calculate specific fuel consumption (g/kWh) and return trip fuel consumption (t/journey), a similar method to that described by Kim et al. (2020) has been adopted, both particular to the vessel's

propulsion system at 85% load factor. The number of journeys required was distinct for each type of vessel (given a 90% carrying capacity) and export demand. BOG losses were considered for LH₂ and NH₃ as both fuels and energy exports.

4.2.2.5 Other energy demands

Iron ore mining and water desalination are additional external energy demands excluded from Homer Pro modelling as they are not considered unique to the decarbonised steel system assessed in this study. Ore mining and processing energy demand was taken from literature as 0.11 MJ/t ore (Talens Peiró & Villalba Méndez, 2013).

Considering global water stress (Schlosser et al., 2014), especially in the Pilbara region (McFarlane, 2015), surface water supply is constrained and desalination is deemed a requirement for all cleaning, process, and cooling water within the supply chain. Although desalination may not be necessary for process cooling water if antifouling treatments are applied (Rubio et al., 2015) or electrolysis if technology becomes more adaptable (Tong et al., 2020), it was consistently applied across all water demands to produce a conservative estimate of energy consumption. Desalination energy demand of 5kWh/kL was taken from the 140,000m³/day Perth Seawater Desalination Plant (Water Technology, 2021).

4.2.2.3 Economic assessment

A standard NPV method was used for calculating the LCOS and LCOH for each case over the 20-year project economic lifetime. The real discount rate was 7% given an annual inflation rate of 1.65% (2016-2020 average, Reserve Bank of Australia (2021)). Costs were originally equalised on an Australian Dollar (AUD) 2020 basis for the published article, but then converted to USD to match the currency used throughout this thesis using a conversion rate of 0.65 USD/AUD. CAPEX included steel plant, electrolyzers, CGH₂ plant (compressor and storage tank), LH₂ plant (liquefier and storage tank), NH₃ synthesis plant (air separation unit, Haber-Bosch process, and storage tank), NH₃ cracker and stationary fuel cell stacks. OPEX included electricity, ship charter (which excludes fuel as it is always derived from electricity), iron ore, labour, water, and infrastructure maintenance (2% of CAPEX). The costing approach treated electricity and shipping charter as externally procured resources since in principle, they need not be explicitly built for decarbonised steel and are more simply expressed in a \$/unit basis. Homer Pro modelling determined the LCOE as well as the energy system infrastructure CAPEX. Charter rates were determined based on the vessel, propulsion system and fuel storage CAPEX plus the OPEX of crew, port fees, consumables, maintenance, repair, and insurance. LH₂ or NH₃ shipping fuel production was incorporated within the overall energy system demands. For detailed economic modelling data and equations refer to Supplementary Methods (of Appendix II).

Fuel cells costs are expected to improve simultaneously with efficiency and lifetime. Stationary SOFC cost data was given by Whiston et al. (2019) who evaluated U.S. DOE targets, with lifetimes up to 90,000 hours (IEA, 2015) assumed for 2030 and an increase to 100,000 hours for 2050. For long-haul mobile FC applications, the U.S. Department of Energy targets of 25,000-30,000 hour lifetime and US\$80-60/kW from 2030 to 2050 (Marcinkoski et al., 2019) were utilised, however these are in

reference to mobile H₂-PEMFC stacks. For mobile NH₃-SOFCs, a hybrid approach has been taken for data selection to make the best use of available data; equal lifetime (and efficiency) as mobile PEMFCs, with equal costs as stationary SOFCs which is more representative of the technology's financial burden. Any improvement in lifetime positively affected the overall cost by reducing frequency of replacement within the project lifetime.

4.3 Results and Discussion

In this section, the energy consumption, and financial costs per tonne of green steel are first presented, then those for establishing and operating the entire system. This is followed by more detailed insights from energy and cost perspectives before further issues are discussed.

4.3.1 Energy intensity and levelised cost of green steel

The two key outputs from the assessment – energy and cost demand of fossil-free steel – are firstly summarised overall and then compared to fossil-based steel.

4.3.1.1 Results overview

The analysis determined that, depending on the case, one tonne of steel in 2030 will demand 5.4-8.6 MWh of electricity and cost \$593-835, reducing in 2050 to 4.9-7.6 MWh and \$465-616. Across all the studied cases, significant improvement in the resource intensity and the levelised cost of fossil-free steel was projected with increasing supply chain concentration in Australia, as shown in Figure 4.3. Thanks to the co-location of energy and steel production, SC3-LH₂ and SC3-NH₃ were the optimal cases which are closely aligned due to the minor influence of shipping fuels and energy vectors. On average, steel produced via SC1 (iron ore and energy exports) and SC2 (HBI and energy exports) were 45% and 19%, respectively, more energy intensive than SC3. Clearly, the additional energy-consuming processes for LH₂ and NH₃ production in these supply chains with greater transport requirements and energy conversion losses burdened the resource systems. By using LH₂ instead of NH₃ for SC1, energy consumption was reduced by 12% in 2030 and 17% in 2050 with costs reduced to about 8% in 2030 and 5% in 2050. Compared to 2030 and depending on the supply chain and energy vector, process efficiency improvements realised in 2050 reduced energy consumption by 9-17%, while the combined effect of lower energy consumption (due to the improved efficiencies) and technology cost reduction led to the reduction of the levelised costs by a more substantial 21-26%. In particular, LH₂ energy consumption dropped markedly due to the projected improvement of liquefaction efficiency.

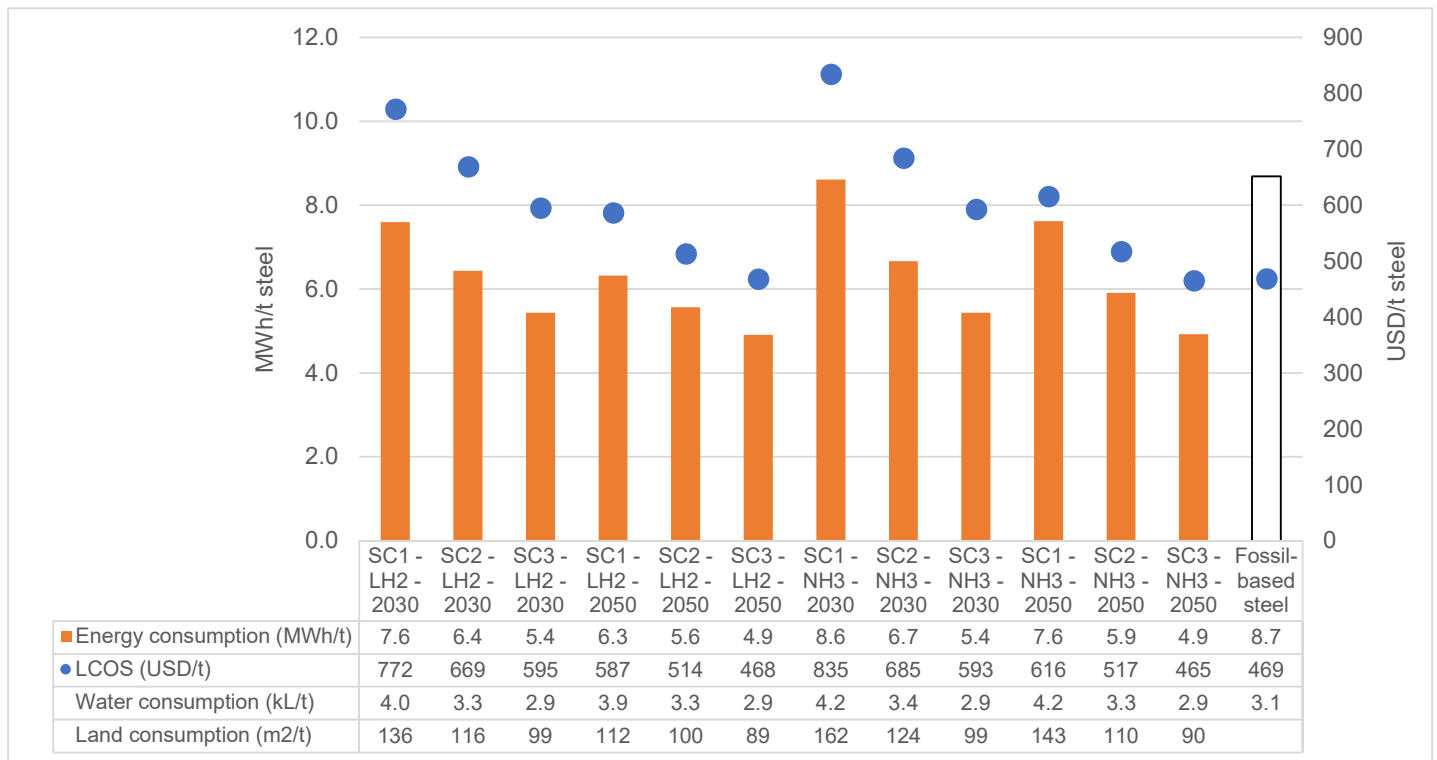


Figure 4.3 Energy demand and financial cost per tonne of semi-finished steel.

The results demonstrate that co-location of mineral and energy inputs with manufacturing processes positively benefits the system in terms of energy and cost efficiency. This suggests that strategic supply chain design is advantageous to investors and customers alike to decrease costs and accelerate market competitiveness.

4.3.1.2 Comparison to fossil-based steel

Commercial fossil-based primary steel is resource intensive. Considering raw material acquisition, iron and steel manufacturing, and related transport (lifecycle assessment modules A1-A3), one tonne of average Australian hot-rolled steel using the BF-BOF route emits about 3 t CO₂ and consumes 9 MWh of energy (BlueScope Steel, 2020; Liberty Primary Steel, 2020). According to the best case predicted in this study, (green) hydrogen-based steel supply chains can remove the carbon emissions arising from fossil fuel powered operations whilst limiting energy consumption to 5 MWh (the energy for hot rolling which proceeds casting is additional, although a relatively minor contributor). These results rely on spatial proximity between renewable energy resources, iron ore deposits and the H₂-DRI-EAF plant, as well as the realisation of projected technology development from 2030 to 2050.

Today's price of steel is highly volatile, yet it can be approximated at \$470/t for semi-finished products (Steelonthenet.com, 2021). Hydrogen-based steel can reach price parity by 2050 for the two optimal cases with Australian-based iron and steel production (SC3). Exporting energy and HBI (SC2), or energy and iron ore (SC1), from Australia reduces the likelihood of market competitiveness. In 2030, a regional carbon price between \$43 and \$125/t CO₂ will be necessary to make green steel competitive

(based on the average 3t CO₂/t steel emitted from Australian produced primary steel). In 2050, the prospective carbon tax threshold is reduced significantly to, on average, \$45/t CO₂ for SC1, \$15/t CO₂ for SC2, and diminishing to zero for SC3.

4.3.2 Overall energy and financial burden of establishing and operating the decarbonised steel supply chain

The scale of the decarbonised solution for an annual throughput of 40 Mt is considerable. The system energy requirements are 195-343 TWh per year, ranging from the most (SC1-NH₃-2030) to the least (SC3-LH₂-2050) demanding cases. This constitutes 74-129% of Australia's total electricity production (DISER, 2020a). In terms of physical capacity, 126-230 GW solar PV panels, 48-96 GW of electrolyzers, and 2-3 desalination plants (operating at 140 ML/day) will need to be installed.

GW-scale energy interventions demand billion-dollar investments. As shown in Figure 4.4, in 2030, the magnitude of capital for SC3 (\$131 billion) is advantageous compared to SC2 (mean 23% increase) and SC1 (mean 56% increase). By 2050, SC3 capital demands shrink due to reducing technology costs by 32% to \$89 billion, facilitating widespread investments and access to commercial markets. On average, 50% of initial capital is required for the solar power plant, 48% for the H₂-iron-steel plant and a minor 2% for the shipping vessels (which excludes fuel cell replacement costs due to negligible influence, as well as water desalination and ore mining CAPEX).

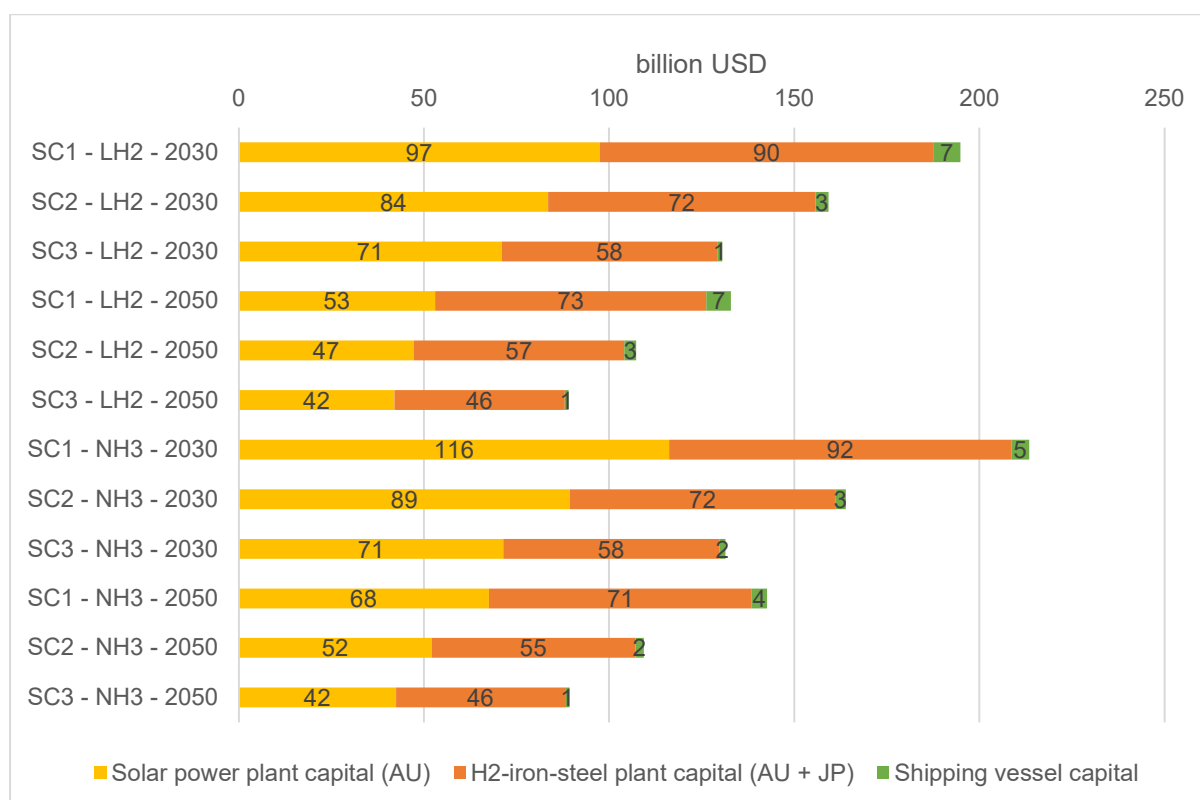


Figure 4.4 Financial capital required to enable 40 Mtpa of H₂-DRI-EAF steel production, split into energy and production, and transportation requirements.

In the comparison of energy vectors, LH₂ cases need less capital than NH₃ equivalents, mainly due to reduced solar power capacity, a relationship most prominent in SC1 with 16% solar CAPEX reduction in 2030 and 21% reduction in 2050; benefits of LH₂ systems increase with time as liquefaction efficiency improvements are realised. Similarly, SC2 solar CAPEX reduces by 7% in 2030 and 9% in 2050 in favour of LH₂, although SC3 differences are negligible. In contrast, fewer liquefied gas tankers are needed for NH₃ due to improved volumetric energy density, reducing the shipping vessel CAPEX.

The above results show the significant energy and financial stress caused by a production system of this scale. To mitigate this stress, supply chains with co-located iron and steel manufacturing, renewable energy and iron resources should be the foremost priority, coupled with the choice of energy carrier based on quantitative evidence. Despite the investment cost reductions acclaimed in 2050 compared to 2030, the decarbonised system requires investment in the next decade to avoid carbon lock-in. This would mean a large financial barrier to be tackled, a challenge further compounded by the consideration of investment losses on existing fossil-based assets.

4.3.3 In-depth examination of energy consumption

Sankey Diagrams were developed to illustrate energy distribution flows; renewable electrons travelling from VRE (start node) to processes based in Australia (light blue nodes) and Japan (dark blue nodes). 2030 cases (Figure 4.5) follow very similar relationships to 2050 cases (see Figure S4.2), although with benefits of process efficiency improvements for electrolysis, liquefaction, and fuel cells. In each diagram, one can see, from left to right, how the VRE was consumed directly by processes that operate in Australia during VRE_{on} and how subsequently the energy flows were re-distributed towards (1) those processes operating in Australia during VRE_{off} (in all SCs except SC1-LH₂), (2) shipping (in all SCs) and (3) the processes operating in Japan (in SC1 and SC2). In all the cases, the centrality of electrolysis is evident in energy consumption, as expected, although diminishing in significance with time (2030 to 2050) and supply chain (SC1 to SC2 to SC3). With LH₂, new energy cost was incurred by the introduction of CGH₂ when moving from SC1 to SC2 due to the operation of the (inflexible) DRI process in Australia, but the overall energy cost for energy vector production and for transport was significantly reduced; this trend contributed when moving from SC2 to SC3. On the other hand, the inflexibility of NH₃ synthesis, in the NH₃-based cases, increases the energy storage (CGH₂) requirement in coping with VRE. Furthermore, Japan-based processes (i.e., dark blue nodes which include energy to carry out processes, and the shipping fuel to transport energy to, Japan) drive up energy demand, especially prevalent for DRI in SC1-NH₃ where NH₃ cracking is also required. These extra energy costs made LH₂ a more efficient energy vector overall, even though NH₃ as an energy carrier required fewer vessel-trips for transporting energy from Australia to Japan (thanks to its 1.7-times greater volumetric energy density) and suffered lower BOG losses than LH₂.

Figure 4.6 further compares the intermediate- and end-users across the 12 cases. The end-use categories cover production feedstock (reductant for DRI), major production energy (EAF, H₂ heating pre-DRI), minor production energy (H₂ compression pre-DRI, casting, iron ore mining and water desalination) and shipping fuel (transport). Intermediate processes cover CGH₂ storage in Australia,

and H₂ liquefaction/NH₃ synthesis for exports and shipping fuel. For each category, energy consumption represents either direct consumption of VRE (for processes running in Australia during VER_{on}), the VRE consumed for producing the portion of H₂ that eventually gets consumed in the category (processes running in JP and transport), or a combination of both (processes running in Australia during both VRE_{on} and VRE_{off}). The most energy-intensive end-use processes are DRI (using H₂ as the reductant) and EAF, representing on average 41% and 28%, respectively, of total demand. If DRI reductant and pre-DRI processes (H₂ compression and H₂ heating pre-DRI) were incorporated, the complete DRI process contribution would increase to 53% (not shown in the chart). From 2030 to 2050, gains in electrolyser, liquefaction and fuel cell efficiency reduce energy demand appreciably.

Further, H₂ liquefaction/NH₃ synthesis constitutes an average 15% of total energy demand for SC1 where energy exports are deeply depended on, diluting to 7% for SC2 and 1% for SC3. H₂ liquefaction, as an isolated process, is initially more energy intensive than NH₃ synthesis as efficiency improvements have not yet been realised; SC1-LH₂ sees relative reduction in energy demand from 19% of total in 2030 to 13% in 2050 (whilst NH₃ stays at 13%). However, SC1-NH₃ requires cracking pre-DRI; summing such energy demand (absorbed in the DRI portion in Figure 4.6) to the burden for synthesising the energy vector increases accountability for these cases (2030 and 2050) to 21%. Transport (i.e., shipping fuel) is a minor overall contributor (average 5%) with any changes mainly due to the transportation of energy (LH₂ or NH₃) as opposed to material. This is due to negligible differences in material export demands between supply chains; iron ore, HBI and steel all require approximately 5 kg H₂/t steel (in the form of LH₂ or NH₃) for dry bulk carrier fuel.

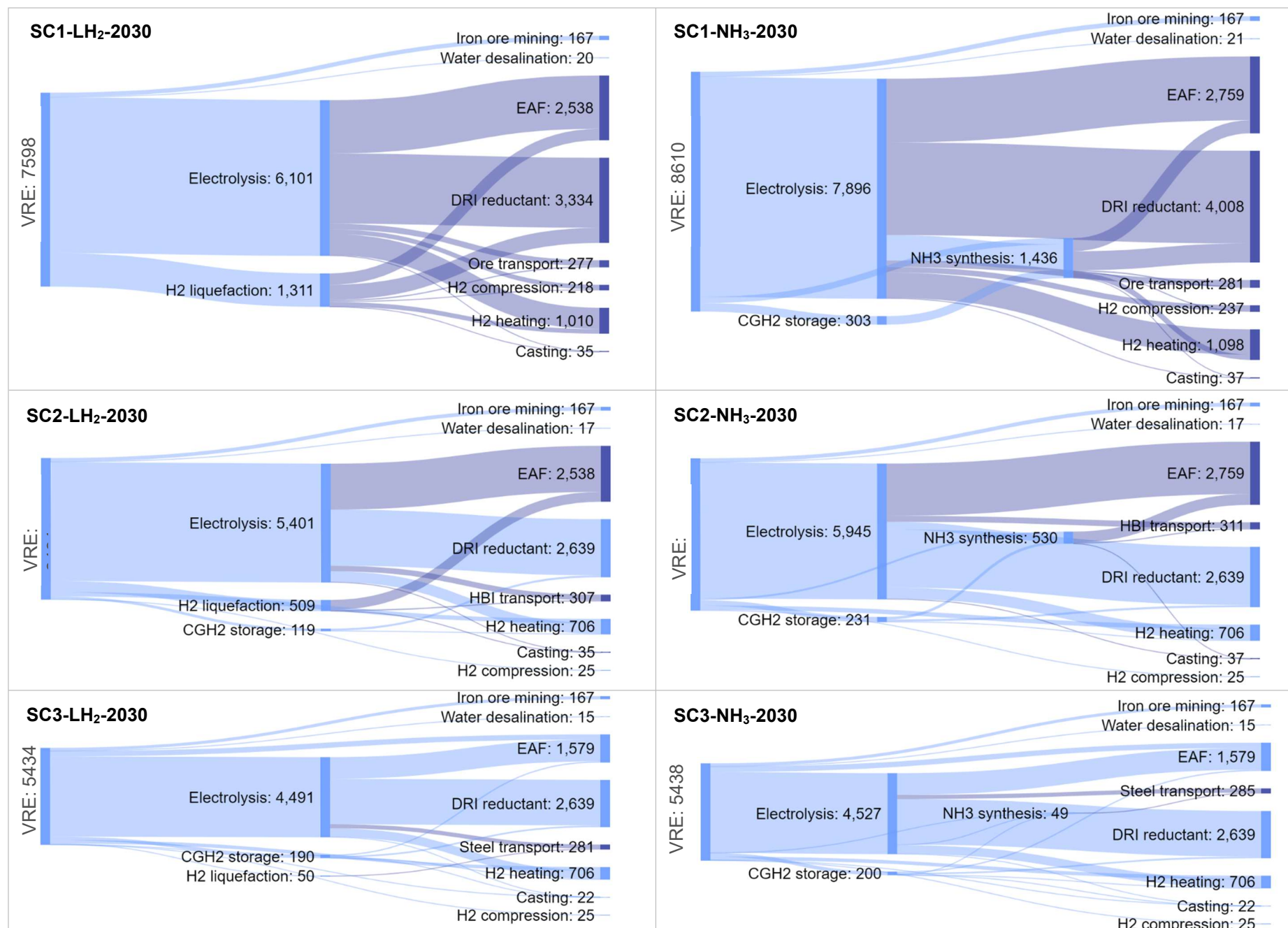


Figure 4.5 Sankey energy distribution diagrams for 2030 cases (refer to Figure S4.2 for 2050 cases)

Note: data in kWh/t steel; may not sum due to rounding to nearest whole number; node width correlates to magnitude of energy demand; scale is normalised for all cases.

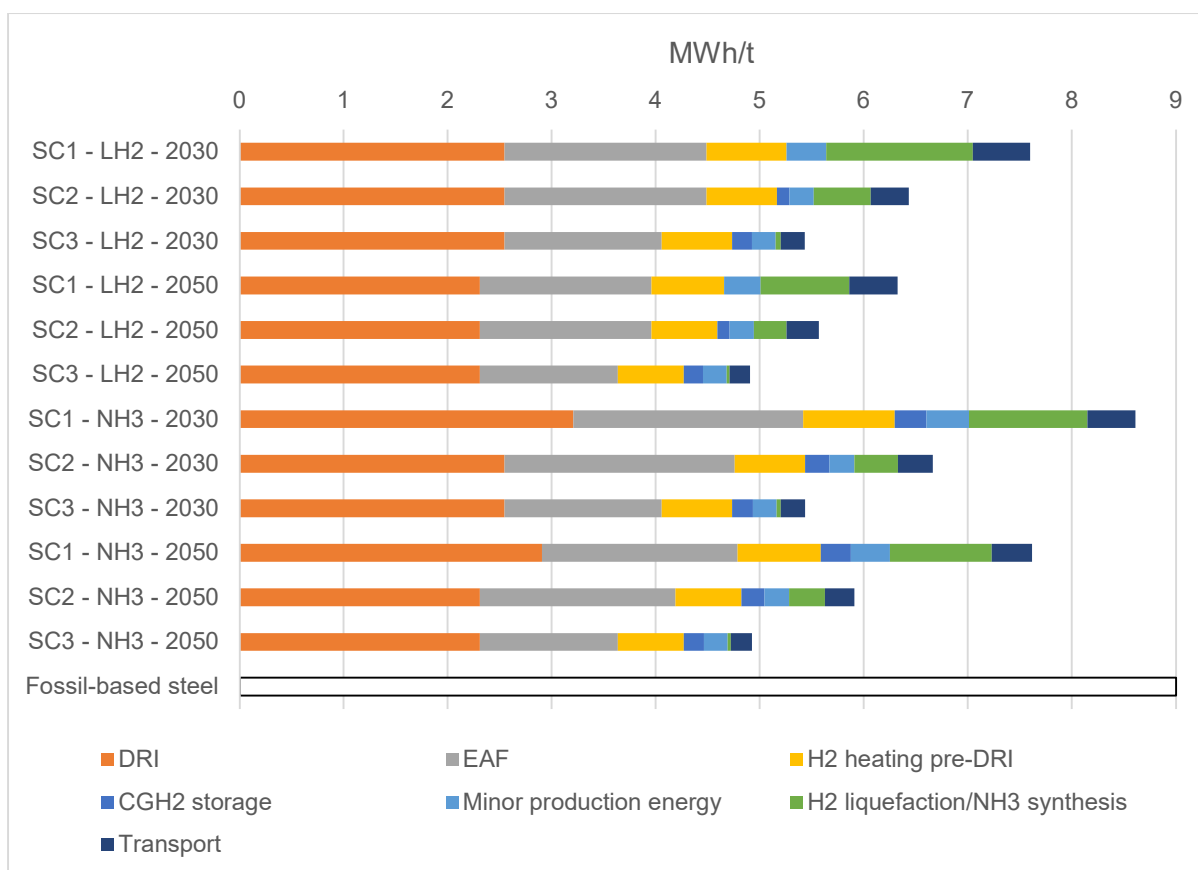


Figure 4.6 Energy consumption for each case across the complete Australia-Japan supply chain, separated by individual processes (MWh per tonne of semi-finished steel).

Pathway process efficiency, from VRE to end-use application, can demonstrate the degree to which LH₂ is advantageous over NH₃ (as shown in Table 4.2 for the major end uses). Inflexible NH₃ synthesis calls for intermediate CGH₂ storage and fuel cells to provide power in non-daylight hours (62% of the day) and using NH₃ as a H₂ carrier demands cracking pre-DRI, driving up process inefficiency. The efficiency gap increases in 2050 due to the substantial reduction in energy demand projected for H₂ liquefaction (down 40%).

Table 4.2 Pathway efficiencies for the most energy-demanding end-use processes in the H₂-DRI-EAF production route, considering various supply chain configurations (MJ VRE required/MJ delivered to end-user).

	Production in Australia		Production in Japan - LH ₂ exports		Production in Japan - NH ₃ exports	
	2030	2050	2030	2050	2030	2050
DRI (H₂ reductant)	66%	72%	52%	61%	43%	48%
EAF	48%	54%	30%	37%	27%	32%
H₂ heating pre-DRI	63%	68%	44%	52%	41%	45%

In summary, the detailed analysis of energy consumption shows the relative importance of different components in the supply chain and how their locations affect their energy demands, with the latter shaped in part by the comparative performance of the two energy vectors which itself is also affected

by the supply chain configurations. Overall, these results show that energy losses are gross for both energy vectors in the processes located in Japan, and that co-location of renewable electrons and H₂-iron-steel manufacturing plant delivers immediate energy efficiency benefits.

4.3.4 In-depth examination of economics

4.3.4.1 Levelised cost of steel

The LCOS for each case is shown in Figure 4.7, separated by key expenditures comprising ~25% CAPEX (infrastructure) and ~75% OPEX (iron ore, labour, water, electricity, shipping, and plant maintenance). The energy-intense nature of the hydrogen-based steel production supply chains is reflected in the costs; electricity accounts for 28-43% of the total. This exceeds current fossil-based production where 20-25% of total costs are required for energy (Horvath, 2013), indicating a shift in revenue dynamics; cheap renewable electrons are central to profitable fossil-free steel. Absolute electricity costs ranged from \$130/t (SC3-2050) to \$360/t (SC1-NH3-2030), depending on the electricity demand and LCOE. The results closely correlated with literature; Wood et al. (2020) estimated hydrogen-based steel, shipped as a semi-finished product from Australia to Japan (i.e., SC3) in an arbitrary future year, to be \$609/t, very close to this study's average SC3-2030 cost of \$594/t.

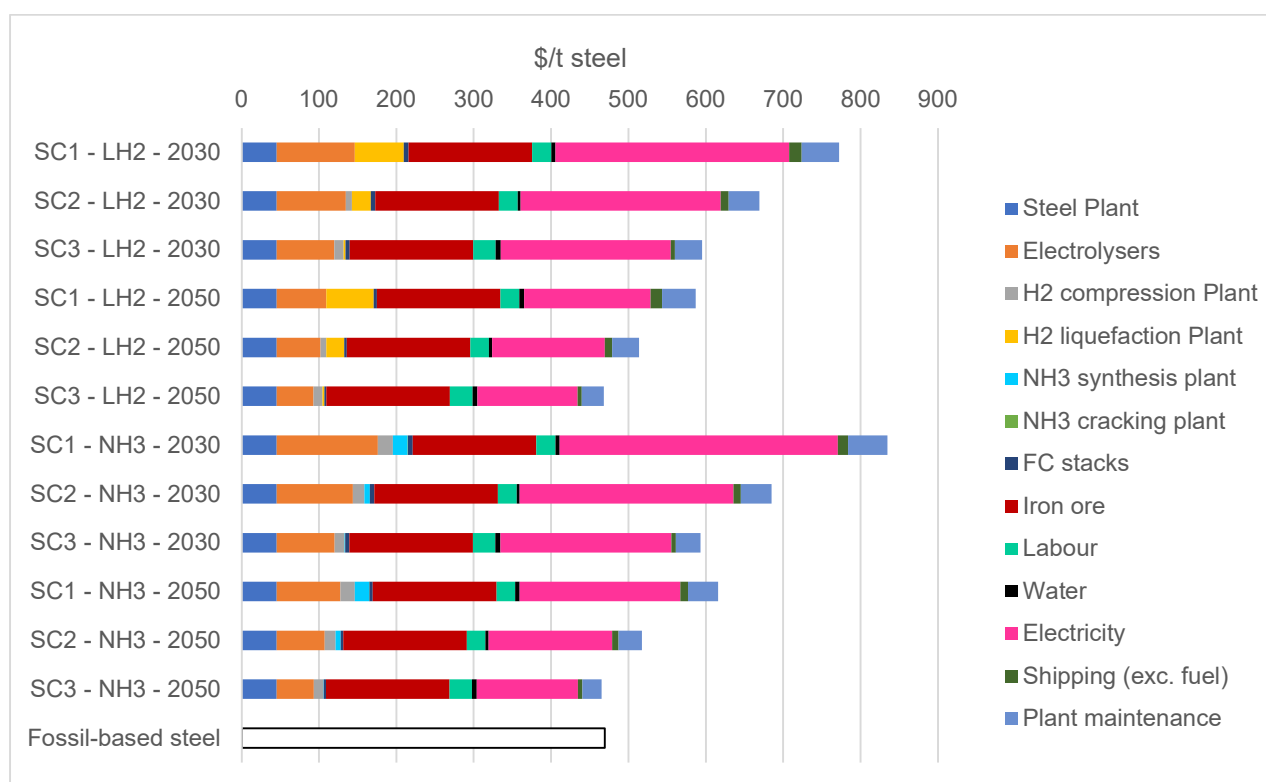


Figure 4.7 Levelised cost of steel for each case of the Australia-Japan binational supply chain (in USD per tonne of semi-finished steel). Note that NH3 plant CAPEX is negligible, such that it cannot be deciphered on this graph.

For CAPEX, electrolysers were the dominant cost factor, accounting for 12% of costs on average, a function of hydrogen demand, electrolyser efficiency and electrolyser unit cost. Influentially, electrolyser efficiency improved by 10% and unit cost reduced by 35% from 2030 to 2050. Regarding hydrogen

demand, SC3 consistently required 0.09t H₂/t steel which increased to an average of 0.11t and 0.014t for SC2 and SC1, respectively. Additionally, NH₃ consumed 29% more hydrogen than LH₂, decreasing to 10% and 1% for SC2 and SC3, respectively.

In terms of H₂ conversion and storage, NH₃ supply chains were more energy-intense however less capital-intense than LH₂ equivalents (encompassing CGH₂, LH₂ and/or NH₃ plant). For SC1, the average LH₂ case dedicated 9% of costs to H₂ conversion and storage infrastructure, compared to 5% for the NH₃ case. CAPEX differences reduced with dilution of export demands, equalising at 3% of total costs for both energy vectors in SC3.

Regarding OPEX, iron ore maintained a constant value of \$160/ steel t across all cases, accounting for 19-34% of the total. Note that market ore prices are highly volatile however will uniformly affect all cases. Plant maintenance, labour, shipping, water, and fuel cell stacks accounted for, on average, 6%, 3%, 2%, 1% and 1% of total cost.

4.3.4.2 Levelised cost of electricity

The LCOE computed using Homer Pro and CSIRO projection data for solar CAPEX (Graham et al., 2020) was on average \$38/MWh for 2030, which decreased appreciably to \$25/MWh for 2050 with solar PV panel cost reduction (down 66%). In comparison, the LCOE computed by Graham et al. (2020) for utility-scale solar PV with similar CAPEX projection data was \$20-36/MWh in 2030 and \$16-29/MWh in 2050. The difference between these LCOE estimates is mainly due to the capacity factor of solar PV installation. In this work, the underlying capacity factor values were calculated by Homer Pro energy modelling specifically for the case study location, which was 21% on average (based on 22 years of historical solar irradiation data in the Pilbara), whereas the low-range LCOE values from Graham et al. (2020) were determined using a higher capacity factor of 32%. Nevertheless, the sensitivity of the LCOE to this study's results was limited; if the LCOE did decrease by 10%, the LCOS would decrease by approximately 3%.

The relationship between electricity demand, process flexibility and variable solar supply altered the LCOE between supply chains and energy vectors marginally; the higher the storage capacity during daylight hours as a percentage of daily load, the greater the flexibility available to the VRE system and hence lower the LCOE. The optimised case was SC1-LH₂-2050 at \$24/MWh, reflecting the most flexible system with competitive solar panel costs. LCOE was slightly improved for LH₂ cases, reduced in comparison to the NH₃ equivalent by 5% and 3% for SC1 and SC2, respectively, then diminishing to 0% for SC3.

4.3.4.3 Levelised cost of hydrogen production

The optimal hydrogen production costs exceeded the Australian government's 'H₂ under \$2' goal (DISER, 2020c), which correlates to \$1.3/kg H₂ in USD. Although, 40% reduction is witnessed over two decades; \$3.1/kg H₂ in 2030, down to \$1.9/kg H₂ in 2050. The slight variations between supply chains and energy vectors echoed trends in LCOE. Costs were dominated by electricity (65%) and electrolyser CAPEX and maintenance (33%), the remaining due to water and labour. 2050 cases evidently benefited

from the reduction of electrolyser CAPEX (down 28%) and LCOE (down 35%) yet costs on a 'per unit' basis were still rather high due to the limited electrolyser utilisation rate of 37.5%. The relationship between daily hydrogen demand and rated electrolyser capacity is critical: an improved electrolyser utilisation rate drives down costs; however, it is only achievable in a region with optimal, more evenly distributed diurnal renewable energy.

4.3.5 Further discussion

The above results and discussion have focused on energy, however, the sheer scale of the green steel production assessed in this work means other resources, particularly water and land, could also be impacted. A preliminary understanding was thus developed of the system's water and land consumption (see Figure S4.3). The processes demanding the greatest amount of water were electrolysis, consuming 9L/kg H₂, as well as the EAF and continuous caster, consuming 1.6kL and 1kL/t steel, respectively (IEAGHG, 2013; worldsteel, 2020c). Net consumption was offset by return water received during DRI and FC power production, if co-located with water electrolysis. This resulted in an annual water demand of 115-169GL across Australian and Japanese operations (depending on the case), equivalent to 80-118% of the Pilbara region's water consumption (based on the most recent available data from McFarlane (2015)). Following a similar method, the system's land footprint was calculated with the dominating footprint from solar panels, quantified at 28 km²/GW, largely determining the results. Based on Australian operations (due to the unifying system condition of energy production in Australia), the system's land consumption was determined to be 3500-6400km² (depending on the case), equivalent to 0.7-1.3% of the Pilbara region's land area. Whilst this footprint is not technically an issue considering Australia's large land mass, it would require consideration in Japan as its entire area as a country is 25% lower than the Pilbara region (Japanese Ministry of Land, Infrastructure, Transport and Tourism, 2007; Pilbara Development Commission, 2021). The range of results for both water and land consumption followed the same trends as energy consumption; co-location of production processes and renewable energy resources reduced system burden, as did the use of LH₂ over NH₃, and 20 years of technology development to 2050. It should be noted that land costs were not considered in the economic model however are likely to follow the trends of land consumption. Moreover, securing renewable energy sites in optimal locations with sufficient land area and water resources are crucial first steps in operation establishment. Limiting production system stress placed on finite water and land resources is supported by localised, energy-efficient supply chains.

There is inevitable uncertainty in dealing with future scenarios and simplifying model assumptions. The accuracy of the energy and economic model is contingent on the accuracy of original data projections. To reduce errors, recent data from reputable organisations and authors were sought and compared, whilst various processes were modelled from first principles using Aspen Plus. Furthermore, the inclusion of two timelines (2030 and 2050) effectively allowed the assessment of the impact of several technical and economic parameters that were projected to improve over time. To gain a deeper understanding of the impact of various independent variables on the dependent variables including energy consumption and LCOS, a sensitivity analysis was conducted of key process efficiencies for 2050 cases, all varied $\pm 5\%$ from the base case (see Figures S4.3 and S4.4). Electrolysis efficiency was

found to be the most influential on both energy demand ($\pm 4\%$ on average) and LCOS ($\pm 2\%$ on average) across all supply chains, followed by fuel cell efficiency (average $\pm 2\%$ energy and $\pm 1\%$ LCOS). Due to energy vector significance, SC1 was most sensitive to liquefaction efficiency ($\pm 3\%$ energy and $\pm 2\%$ LCOS), reducing in impact for SC2 ($\pm 1\%$ energy and $\pm 0.5\%$ LCOS) to almost nil for SC3. Similarly, SC1 was most sensitive to NH_3 synthesis efficiency though to a lesser extent ($\pm 1\%$ energy and $\pm 0.5\%$ LCOS), reducing to approximately zero for SC2 and SC3. Reflecting on these uncertainty ranges, the differences between NH_3 and LH_2 for SC3 are considered negligible for SC3 ($\pm 0\%$ energy, 1% LCOS), however still visible for SC1 ($\pm 14\%$ energy, $\pm 6\%$ LCOS) and SC2 ($\pm 5\%$ energy, $\pm 1\%$ LCOS). If LH_2/NH_3 process efficiency variation exceeded $\pm 5\%$ from the assumed data points, resultant energy vector relationships may change. For each of the 12 cases the LCOE varied only marginally during the sensitivity analysis, due to the largely unchanged ratio of storage capacity to daily load (representing VRE system flexibility).

Several other assumptions adopted by this study warrant further discussion. Firstly, the range of DRI products – hot-DRI, cold-DRI and HBI - should be considered in detail, including the distinct energy burdens and transportation challenges. This study omitted the additional energy burden of HBI pre-heating in the EAF based on the assumption that this requirement could at least in part be met by the recycled heat from the EAF. Nevertheless, this omission could lead to slight underestimation of (but without affecting the qualitative conclusion on) the advantages acclaimed from co-locating DRI and EAF facilities. Secondly, “Instant” establishment of the decarbonised supply chains was assumed at each of the two timelines. A transition period will be needed instead of a sudden switch, which can have important implications in terms of investments and the deployment of technical facilities and have not been considered in this work. It should also be noted that system efficiency could be improved by improving the operational flexibility of those processes considered here as inflexible, through better synchronisation between VRE supply and manufacturing as shown in other renewables-driven processes (Chen & Yang, 2021). Finally, BOGs were accounted for as mass losses. However, they could be contained using an integrated re-liquefaction system, where energy is required to re-liquefy the gas and send it back to the tank as a cool liquid (Ahn et al., 2017); energy losses estimated for such a system may deviate from the mass losses considered here, although the impact to the overall energy efficiency is unlikely to be significant.

4.4 Conclusions

In this study, 12 unique green H_2 -based steel supply chains were simulated, differentiated by spatial configuration, timeline, and energy carrier. Results demonstrated that direct energy and ore exports to remote steel producers (i.e., Japan-based production), as opposed to co-locating iron and steel production with abundant ore and renewable energy resources (i.e., Australia-based production), increased energy consumption and the cost of steel by 45% and 32%, respectively, when averaged across 2030 and 2050. Two decades of technological development and economies of scale realisation would be crucial; 2030 supply chains were on average 12% more energy-intensive and 23% more expensive than 2050 equivalents. On energy vectors, liquefied hydrogen was more efficient than

ammonia for export-dominant supply chains due to the pairing of its process flexibility (compared to the inflexible Haber-Bosch process) and the Pilbara's intermittent solar energy profile, as well as the avoidance of the need for ammonia cracking prior to direct reduction. To mitigate the green premium, a carbon tax in the range of \$43-125/t CO₂ would be required in 2030 and \$0-45/t CO₂ in 2050; the negligible carbon tax requirement in the latter is achievable only by Australia-based steel production. Further, the modelled system scale was immense; producing 40Mtpa (Japan's 2050 steel demand) of decarbonised steel will require 74-129% of Australia's current electricity output and \$89-213 billion in capital investment for solar power, production, and shipping vessel infrastructure.

Chapter 5. Green Steel Transitions

Overview & Motivations

This chapter presents the following unpublished manuscript (currently under review by a journal): Devlin, A., Mykhnenko, V., Zagoruichyk, A., Salmon, N., & Soldak, M. (2024). Techno-economic optimisation of steel supply chains in the clean energy transition: a case study of post-war Ukraine. The corresponding Supplementary Information is contained within Appendix III.

Among all authors who contributed to the research, A.D. conceptualised the study, developed the supply chain optimisation model, analysed the results, wrote and revised the manuscript, V.M. supported with the conceptualisation, developed the economic multiplier model, and contributed to writing of the manuscript, A.Z. supported data collection and analysis, and contributed to writing of the manuscript, N.S. developed the green electricity and hydrogen optimisation model, and contributed to writing of the manuscript, and M.S. supported data collection and analysis. The GAMS code developed in this study by A.D. for the steel production and trade optimisation model is available online, alongside the input data files (<https://doi.org/10.25446/oxford.24146466.v1>).

This third piece of original research combined aspects of the previous two studies – facility-level optimisation and supply chain assessment – to deliver a sophisticated supply chain optimisation study. In narrowing the spatial scope (from global, to regional, and now national), the network of mass and energy flows could be studied in detail and feasible sectorial green steel transition strategies evaluated. The research strived to determine the optimal iron and steel production and trade strategy for a transitioning economy with large coal-based asset fleet, as well as the enabling financial and natural resources. Some critical modelling developments transpired, including an increased spatial resolution to 1°x1°, introduction of existing asset inertia accounting, inclusion of a diverse mix of energy sources and technology archetypes, and extension of the national demand profile to include regional green HBI and steel exports. At the core of the analysis is a spatially granular green steel transition optimisation model which utilises the outputs from a cost-minimised renewable energy, green hydrogen, and green ammonia production model. The broad requirement for continuous DRI operations was shown in previous work (Chapter 3) to limit the benefits of EAF flexibility, so at facility-level, this study focuses on optimising energy inputs. Subsequently, optimal sectorial supply chain networks are explored, focusing on plant locations, technology, and fuel selection. The contextual framing of post-war Ukraine was both timely and important, wide destruction of iron and steel production and transportation assets, anticipated rebuilding funds. Ukraine was selected as the case study for its regional significance, anticipated EU accession, iron ore resources, extensive steelmaking history, and the added necessity for industrial regrowth given its shattered economy, high unemployment, and destroyed iron and steel assets. Additionally, Ukraine's high green steel market potential was already demonstrated in the facility-level optimisation model (Chapter 3). We provide a strong case for the adoption of a green steel industrial

recovery strategy, underpinned by a feasible technology investment plan and justified returns on this investment.

5.1 Introduction

On 24th February 2022, Russia invaded Ukraine, a major escalation of the existing Russo-Ukrainian war, which began in 2014 with the annexation of Crimea (Biersack & O’Lear, 2014; European Union, 2022a). Ukraine’s steel industry has been severely affected by the Russian invasion, with deliberate attacks on industrial assets and transport routes, as well as the seizure of hydrocarbon resources in the Donbas region in the east and the Black Sea-Sea of Azov areas in the south (Mykhnenko, 2020). Whilst the war endures, plans have been developed for Ukraine’s post-war recovery to restore stability and stimulate economic growth with a Ukraine Development Fund to draw funds (BlackRock, 2023). Rebuilding the steel sector could include a transition to near-zero emissions. This recovery pathway could potentially be economically competitive with the right investment timing and selection of technologies.

Ukraine’s export-oriented steel industry is fundamental to the national economy, though, it is deeply dependent on fossil fuels. The steel sector has remained the second largest employer within manufacturing, with average monthly nominal wages being 15% higher than the national average (State Statistics Service of Ukraine, 2022). In 2021 (pre-invasion), the steel sector (including ‘Basic metals’ and ‘Fabricated metal products’ industries) accounted for 2.3% of Ukraine’s Gross Domestic Product (GDP) and 14.5% of Ukraine’s industrial output, with steel companies selling \$16bn worth of basic metals abroad, and paying \$3.5bn in taxes to the State budget (Boyko, 2022). Yet, Ukrainian steel production emits copious amounts of greenhouse gas emissions; in 2020, the nation produced 20.6 million tonnes (Mt) of steel, causing 48 Mt CO₂ which was equivalent to 15% of national emissions (318 Mt CO₂; Ministry of Environmental Protection and Natural Resources of Ukraine (2023)). The nation produces some of the world’s most emissions-intensive steel at 2.3 t CO₂/t steel on average – the worst ranking of the 17 studied nations/regions (Hasanbeigi, 2022). There is deep dependence on coal-based blast furnaces (BF), and ongoing use of outdated open-hearth furnaces (OHF), which have been substituted widely by the more efficient basic oxygen furnace (BOF). Of Ukraine’s total pre-war steel production, 76% stemmed from the BF-BOF route, 19% from the BF-OHF route, and 6% from the electric arc furnace (EAF) route (worldsteel, 2021b). The average emissions-intensity for the BF route was 2.41 t CO₂/t steel (Metinvest, 2020), and for the EAF route 0.77 t CO₂/t steel (Interpipe, 2021).

Green steel could offer a practical way forward towards the long-term climate neutrality goal that revitalises economic activities and supports Ukraine’s security aims. Green steel could emerge as an export and investment catalyst, necessitating focused investment in adaptable and innovative production capacities (Sologoub et al., 2022). Furthermore, clean industry investments will support stronger long-term economic and environmental outcomes by creating new green jobs whilst decreasing CO₂ emissions (Zagoruichyk et al., 2023) – especially important as unemployment rates have soared to 25% (National Bank of Ukraine, 2023). The economic case for Ukraine using renewables in steel production also changes under European Union (EU) membership requirements. Attaining

membership in the EU will aid in economic resilience and trade integrity as Ukrainian-EU supply chains converge. In the event of Ukraine's accession to the EU, the country will become subject to the regulatory framework of the Emission Trading Scheme (ETS), wherein the carbon price, as of August 2023, is established at around \$100/t CO₂ (Ember, 2023) and is forecast to increase to \$250/t by 2050 without any free allowances (IEA, 2022). The 'EU Green Deal' targets commercialisation of near-zero emissions steel by 2030 and full decarbonisation of the sector by 2050 (European Commission, 2023). Consequently, Ukraine must prepare for this impending transition. This study addresses the knowledge gap on how to strategise the development of efficient and competitive green steel supply chains, underpinned by strategic regional trade partnerships.

After briefly charting the existing literature on decarbonised steel production technologies and their supply chain configurations, this paper presents the steel supply chain optimisation model, and connecting renewable energy (RE) optimisation model, as well as other core components of the methodology. All potential transitions depend on how the war evolves; hence, this research is framed within two scenarios with distinct geopolitical and natural resource constraints. Following, results are presented and discussed, and relevant conclusions drawn for policymakers, investors, and steelmakers to support the industrial transition.

5.2 Literature Review

5.2.1 Steel decarbonisation options

This study follows a deep decarbonisation framework to assess the economic viability of Ukraine's green steel transition. Ironmaking - where reduction of iron ore to metallic iron and, therefore, most emissions occur - precedes steelmaking - where alloying elements are added to the mix and impurities removed via slag. The ironmaking process can be eliminated for scrap-based EAF production. However, since scrap supply is globally constrained and in especially low supply in developing nations (Wang et al., 2021), enhancing material recyclability will support, but not solve, the steel sector's decarbonisation challenge. Therefore, transformative deep decarbonisation technology for ore-based production is needed to shift the industry onto a near-zero emissions trajectory. If fossil fuels are completely removed from the process as ore reductants and thermal energy inputs, a minor amount of carbon must be added during steelmaking (steel is an alloy of iron and carbon), producing a small amount of CO₂, alongside the CO₂ produced from the graphite electrodes in electric smelting operations, which total less than 5% of BF-BOF emissions (Vogl et al., 2018). Although there is no universal definition of 'green steel' (Hasanbeigi, 2023), the IEA proposed a quantitative threshold for near zero-emissions production of less than 0.4 t CO_{2e}/t steel for 100% ore-based production, reducing linearly to 0.05 t CO_{2e}/t steel for 100% scrap-based production (Levi et al., 2022). Subsequently, 'green steel' is defined in this work as *steel produced in the (near full) absence of fossil fuels*, used interchangeably with 'near zero-emissions steel'. This definition is extended to 'green' hot briquetted iron (HBI), the intermediary product between direct reduction ironmaking and steelmaking.

A variety of technologies within the steel production process can reduce industrial emissions. Three key deep decarbonisation pathways lead sectoral innovation of ore-based production: green hydrogen-

based direct reduction of iron (followed by EAF steelmaking; H₂-DRI-EAF), direct iron electrolysis (followed by EAF steelmaking), and carbon capture, utilisation and storage (CCUS) retrofitted to integrated BF-BOF facilities (Fan & Friedmann, 2021). Considering the dominance of BF assets in Ukraine, H₂ injection, top gas recycling, and bio-carbon integration could also be useful, but all offer only partial emissions reductions. Computational modelling has shown the maximum H₂ injection rate to be 28 kg/t with 12vol% oxygen enrichment, which can reduce CO₂ emissions by 18% (Shatokha, 2022). CCUS has limited effectiveness due to the multiplicity of flue gases in a BF-BOF facility and is not yet proven at industrial-scale. Simultaneous CO₂ capture from BF, power plant, and hot stove gases could reduce total plant emissions by 80%; however, costs and energy consumption for solvent regeneration also increase (Normann et al., 2019; Sundqvist et al., 2018). Fully electrified ironmaking would be a transformative innovation breakthrough: research and development has been intensifying for both molten oxide electrolysis (MOE, operating at 1600°C) and electrowinning (operating at around 100°C) (Cavaliere, 2019). Nonetheless, this technology is in its infancy with commercialisation not expected before 2035 (MPP, 2022).

Currently, the most promising path forward is H₂-based DRI production, a modification to the existing natural gas-based process, which is rapidly approaching commercialisation. Although DRI reactors have not yet surfaced in Ukraine, the DRI route accounted for 8% of global iron output in 2021 (worldsteel, 2022). Swedish companies HYBRIT and H2GS, among others, are in the race for the world's first commercial 100% green H₂-based DRI plant - the former successfully completed a pilot-scale H₂-DRI plant in 2020 and underground H₂ storage in 2022 (SSAB, 2022), and the latter is working towards a commercial-scale plant by 2025 (H2 Green Steel, 2022). The Ukrainian government already sees a push for a green H₂-based steel supply chain as a part of the country's recovery strategy (National Recovery Council, 2022). Hence, green H₂-based steelmaking is poised as the technology that will transform the steel sector and is spotlighted in this study for producing both green steel and green HBI.

In this work, the phase-out of current fossil-based steelmaking alongside the phase-in of low and near-zero emissions steelmaking was explored. Two main transitional technologies were investigated: firstly, the DRI-EAF route using various natural gas (NG) and hydrogen (H₂) blends as the reducing gas. Natural gas-based DRI is a mature technology that supports up to 30% H₂ substitution in the feed gas without any infrastructure changes (Astoria et al., 2022), whilst infrastructure upgrades can support H₂ substitution up to 100% (Vogl et al., 2018). Secondly, since DR shaft furnaces do not support BF-grade iron ore and iron ore supply quality is constrained (Kim & Sohn, 2022), the DRI-melter-BOF route was explored, with an Open Slag Bath Furnace (OSBF) as the melting unit. Adventurously, this route provides a production avenue for lower quality ores and takes advantage of existing BOF assets. The production and trade of HBI as an agent for iron and steelmaking dislocation was also investigated. Regarding energy sources, the Ukrainian sector may build on existing energy infrastructure, which is nuclear dependent with rising solar and wind capacity. Pre-war (in 2021), the nation produced 155 terawatt-hours (TWh), 55% from nuclear, 24% coal, 7% hydro, 7% gas, 4% solar, 3% wind, and 1%

geothermal/biomass (BP, 2022). Hence, in addition to CO₂-free nuclear and hydropower resources, this study explores the upscaling of onshore hybrid solar and wind plants, and offshore wind plants.

High-quality renewable energy, that produces cheap CO₂-free electricity and hydrogen, underpins the business case for green H₂-based steel production (Devlin et al., 2023). Green H₂ is produced via electrolysis - the splitting of water (H₂O) molecules into its constituent elements using renewable electricity. H₂ facilitates iron ore reduction, providing the chemical energy input that replaces coal. Because of its low density, the transport of gaseous hydrogen is very expensive in the absence of a pipeline. In order to ameliorate the transport costs, many projects consider the use of hydrogen derivatives, which are denser than hydrogen and can, therefore, be transported and stored more cheaply. There are several derivatives under contention: liquified hydrogen, green methanol, synthetic green natural gas and green ammonia are all discussed in the literature as potential choices. No clear consensus has formed in the literature so far regarding the best hydrogen carrier. Here, we focus on green ammonia (NH₃) as a potential derivative, as it has several advantages: it is liquid under comparatively mild conditions; it can be produced from only water, power and air, and does not need access to a source of carbon; and it is already synthesised and transported globally in very large volumes. Upon delivery to a steel plant, it can be cracked back into the hydrogen that is required by a DRI (Salmon & Bañares-Alcántara, 2021). To secure the immense quantity of zero emissions electricity and hydrogen required for green steel supply chains, green NH₃ may become a critical supply chain mobiliser.

5.2.2 Techno-economic assessments of green H₂-based steel production

This study sits within the growing repository of decarbonisation literature covering techno-economic locational assessments for green H₂-based steel production, of which the key contributions are detailed in Table 5.1. Most studies have explored ideal locations and/or supply chain configurations given local resource and/or green commodity import availability. Whilst some investigated grid-powered production, others modelled islanded energy systems. Thus far, the geographical focus has been Europe. Existing literature on decarbonising the Ukrainian steel sector is scarce: whilst a broad vision for the sustainable future of Ukraine's steel industry was provided (Shatokha, 2016), the only technology focus was utilising best available technologies in existing BF routes (Shatokha et al., 2020).

Table 5.1 Summary of key literature focused on techno-economic assessments of green H₂-based steel production. The levelised cost of steel (LCOS) production is used as a key economic measure (presented below in equivalent USD).

Source	Location(s)	Method	Findings
Bhaskar et al. (2022)	Norway	Optimisation model of H ₂ -DRI-EAF production with H ₂ and HBI storage, and time-variable electricity prices.	Norway is ideally located near raw material inputs and European green markets, with LCOS estimated at \$622-722/t steel. Procuring electricity from day-ahead markets, compared to a fixed power price, could reduce the LCOS by 15%.
Devlin & Yang (2022)	Australia and Japan	Scenario-based simulation model which varied in supply chain configuration and H ₂ energy carrier (LH ₂ , NH ₃) and forecast to 2030 and 2050.	Co-locating production processes with material and energy inputs will reduce energy consumption by 31% and LCOS by 24% (average from 2030 and 2050 results), when compared to exporting H ₂ and iron ore to intercontinental steel producers. Australia is ideally placed for green iron and/or steel production.
Devlin et al. (2024)	Global	Optimisation model of H ₂ -DRI-EAF production using variable wind and/or solar power, forecast to 2030, 2040 and 2050, with each case repeated 5 times for various historical RE capacity factors (2015-2019).	Low-cost green H ₂ -based steel was located nearby the tropic of Capricorn and Cancer, characterised by superior solar with supplementary onshore wind. By 2050, the most favourable locations had a LCOS of \$535/t and, if coking coal prices remain high, renewables-based steel could attain market competitiveness from 2030.
Lopez et al. (2023)	Germany, Spain, and Finland	Scenario-based simulation model which varied in supply chain configuration and forecast to 2020, 2030, 2040, and 2050.	HBI imports (via ship) are more cost-effective than H ₂ imports (via pipeline) from Morocco. Steel production using HBI imports from Morocco is competitive with local European supply chains. Lowest H ₂ -DRI-EAF costs were in solar-rich Spain with LCOS decreasing from \$512/t steel in 2030 to \$386/t steel in 2050. Especially large potential in Australia and Brazil for green steel production exists due to copious ore resources.
Otto et al. (2017)	Germany	Scenario-based simulation model which varied in technology dependence.	Nation-wide, integration of 237 TWh of renewable electrical power would be required to switch to green H ₂ -based steelmaking, with emissions reducing to 5% of 1990 levels.
Pimm et al. (2021)	UK	Optimisation model of H ₂ -DRI-EAF production using variable wind and/or solar power based on historical RE capacity factors (2000-2019 data used, aggregated to four time-slices per month).	The optimal energy system comprises (oversized) electrolyzers, solar and wind energy, combined cycle gas with carbon capture, H ₂ storage and compressed air energy storage. A portion (e.g. 20%) of dispatchable power allowance is influential in reducing H ₂ storage requirements. Before 2030, the costs of switching to H ₂ -based steelmaking could be less than carbon price forecasts.
Toktarova et al. (2022)	Northern Europe	Scenario-based optimisation model which varied in economic parameters, DR furnace flexibility and steel demand location.	Low-cost electricity is the primary cost driver for location selection of electrified steel plants and may vary from present day sites. Solar and wind capacity growth will best meet increased electricity demand (whilst gas base load reduces).
Trollip et al. (2022)	South Africa	Scenario-based optimisation model for green H ₂ -based DRI production, using solar resources in South Africa and EU electricity market prices.	South Africa could produce green HBI at \$395/t HBI. For steelmaking in the EU to be competitive with HBI imports from South Africa, electricity prices must fall below \$38/MWh.

Wang et al. (2023)	Australia	Geospatial resource mapping assessment followed by an optimisation model of H ₂ -DRI-EAF production using variable wind and/or solar power (under fixed ratios of 100% solar/wind, or 50% each).	Correlation exists between the location of iron ore deposits and high-quality renewables, as in the Pilbara region of Western Australia and Eyre Peninsula of South Australia. Additionally, new steelmaking activities could benefit from existing power and transport infrastructure from mining operations. LCOS estimated at \$500/t steel in 2050.
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5.2.3 Research Gaps

Multiple research gaps can be identified from the summary of current literature. Firstly, the lack of geographical coverage of developing nations nor unstable socio-political contexts. Secondly, whilst plant-level optimisation and supply chain simulation has been explored, supply chain optimisation has not. According to the authors' knowledge, supply chain optimisation is absent in steel decarbonisation literature, where the movement of energy and raw materials to iron and steelmaking production sites, and then onwards to demand markets, is assessed. This study fills the literature gaps by adopting a geospatial explicit optimisation modelling approach and selecting post-war Ukraine as the case study: a nation with substantial iron ore resources and steelmaking capabilities, as well as an urgency for industrial growth given its shattered economy, high unemployment, and destroyed iron and steel assets. This work builds on the authors' previous studies (Devlin et al., 2023; Devlin & Yang, 2022) in three major aspects: (i) expanding the spatial scope to national-level with regional export links, (ii) incorporating existing asset inertia and a range of transitory technology and fuel options, and (iii) moving beyond pure techno-economics by framing the analysis around geopolitical considerations and climate policies. The approach taken enabled a rigorous evaluation of steel supply chain networks on the pathway to near-zero emissions by 2050.

5.3 Methods

5.3.1 Optimising the steel sector's transition to near zero emissions

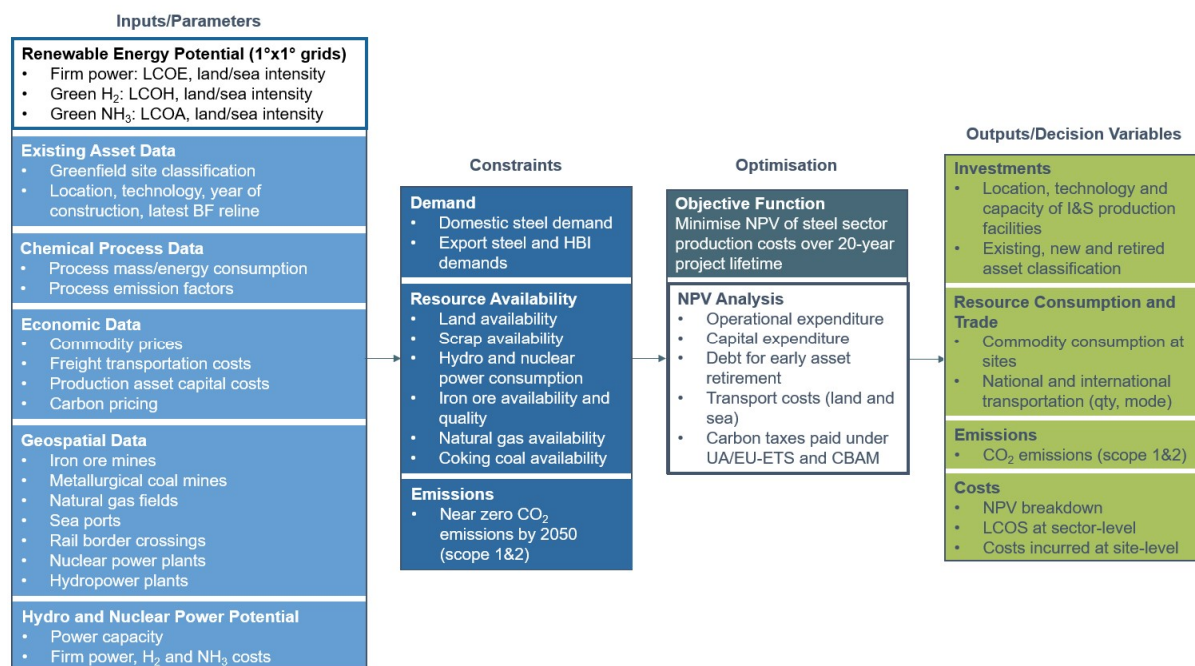


Figure 5.1 Schematic of the green steel transition model.

The supply chain optimisation model utilises spatially granular data to determine where, when, and what iron and steelmaking technology investments should occur, as depicted in Figure 5.1. The model was developed using GAMS (General Algebraic Modelling System) software as a Mixed Integer Linear Programming (MILP) problem. It optimised for lowest net present value (NPV) over the 20-year project lifetime, with a discount rate of 8% using the CPLEX solver. The movement of materials and energy were informed by natural resource constraints (e.g. land availability for installation of RE infrastructure, iron ore reserves, and metallurgical coal reserves), circularity constraints (scrap steel availability), steel demand profiles (domestic and exports) and carbon pricing mechanisms. Possible supply chain nodes included manufacturing sites, ports, rail border crossings, ore mines, metallurgical coal mines, natural gas fields, offshore wind sites, nuclear power plants, and hydropower plants. Importantly, both brownfield and greenfield sites were explored over the entire nation. Refer to Supplementary Methods in Appendix III for detailed model description and equations.

In Ukraine, as defined by the pre-2014 national boundaries, 73 possible iron and steel plant locations and over 100 possible renewable energy production locations were considered at 1°x1° grid spatial resolution (about 111 km (latitude) x 73 km (longitude)). Electricity generation is decentralised - each grid can produce its own renewable power or import electricity/H₂/NH₃ from other grids. Green commodities (electricity, H₂ and NH₃) can be sourced from onshore hybrid solar/wind, offshore wind, nuclear or hydropower plants. This study builds on modelling competencies within previous work (Devlin et al., 2023) for 100% green H₂-DRI-EAF steel production at the facility-level, with important extensions regarding energy source and technology diversification, supply chain integration, carbon policy

economics, and existing asset incorporation. The model was repeated in 2030, 2040 and 2050 with physical asset inertia (i.e., carry-over of installed capacities) and cumulative natural resource consumption (affecting land availability, ore reserves and metallurgical coal reserves). This modelling approach allowed exploration of the interplay between operational costs, capital costs, debt incurred for early furnace retirement, and carbon prices. The inherent uncertainty involved in future energy system modelling, especially in this unstable socio-political context, has been reduced by using detailed local resource and economic input data (as specified in Table 5.2).

Table 5.2 Key data inputs to the supply chain optimisation model.

Data type	Description and source(s)
Existing iron and steelmaking assets	Ukraine's 19 BF's, 13 BOFs, 8 OHFs and 3 EAFs of either operating or mothballed status (GEM, 2023e) were modelled as existing assets, with the exclusion of Mariupol's Azovstal and Ilyich Iron and Steel Works as they are at least partially destroyed, and the extent of damage and restoration requirements are unclear (World Bank Group, 2023). Asset ages and BF relining campaign lives (GEM, 2023a) were used to determine asset depreciation.
RE-based electricity, H₂ and NH₃ production costs and land/sea intensities	The levelised cost of electricity (LCOE), hydrogen (LCOH) and ammonia (LCOA) are outputs from a separate RE optimisation model, which produces green commodities for continuous supply to industrial users. Sea and/or land consumption rates are also determined (refer to Section 5.3.2).
Nuclear/hydropower-based electricity, H₂ and NH₃ production costs	The base price of nuclear/hydropower was assumed to be \$20/MWh based on the historical range in recent years: \$18-22/MWh for hydropower (National Energy and Utilities Regulatory Commission, 2018) and \$18-29/MWh for nuclear power (Accounting Chamber of Ukraine, 2020). Production costs of H ₂ using continuous electricity supply were determined using a simplified levelised cost calculation based on low temperature electrolyzers (refer to SI Table S5.15 for unit costs). Consequently, NH ₃ costs were determined by adding on energy demand and costs for the Haber-Bosch process (refer to SI Table S5.17 for unit costs).
Nuclear and hydropower power capacities	For nuclear capacity, only two nuclear reactors of Ukraine's current fleet of 15 (GEM, 2023d) will still be operational past 2050 based on an expected lifetime of 60 years for newer units (World Nuclear Association, 2022). The model assumes that these two reactors are upgraded to 150% of current capacity, totalling 3000 MW (22% of current capacity), which continue to operate at a capacity factor of 71% (based on 86 TWh of nuclear power produced in 2021 (BP, 2022)). For hydropower capacity, the ten operational plants sum to a combined capacity of 6,247 MW (excluding the destroyed Kakhovka Dam and Hydroelectric Power Plant) (GEM, 2023c). The model assumes a capacity factor of 30% across the existing HPP asset fleet, and that the steel sector can consume 20% of the produced electricity.
Geospatial data	In addition to the grid-level RE potential data and coordinate-level GEM data for steelmaking assets, nuclear power plants, and hydropower plants, geospatial data was integrated for natural gas fields (EITI, 2020), iron ore mines (GMK, 2023a), metallurgical coal mines (Amosha et al., 2017), and sea ports (Shipnext, 2023).
Commodity prices	The most critical energy and material inputs for steelmaking are commodities traded on global spot markets, hence, prices fluctuate significantly over time. Due to the high number of variables already considered in the model, constant prices were assumed based on historical averages: DR-grade iron ore was priced at \$100/t (Black Iron, 2023), BF-grade iron ore at \$80/t (World Bank Group, 2022a), scrap at \$300/t (GMK, 2021), natural gas at \$25/MWh (Eurostat, 2023) and metallurgical coal at \$200/t (DISR, 2023). For the complete list of commodity prices, refer to SI Table S5.25. A sensitivity analysis on these economic inputs was conducted, as shown in the SI Tables S5.1-S5.4.
Freight transportation costs: railway freight (dry bulk goods), pipeline (liquefied NH₃, NG) and power grids (electricity)	The unit cost of dry bulk railway freight was \$0.025/t/km (Forbes, 2022), with 30% fuel consumption reduction considered on the return leg. Pipeline costs for liquefied NH ₃ were \$0.05/t/km (Nayak-Luke et al., 2021) and for NG \$0.08/t/km (DeSantis et al., 2021). The electricity transmission tariff for green metallurgical enterprises of \$5.67/MWh/km was used, as set by the Ukrainian National Commission for State Regulation of Energy and Public Utilities (Verkhovna Rada of Ukraine, 2022). For related equations refer to the Supplementary Methods.

Chemical process data	For selected iron and steel production processes as well as NH ₃ cracking (needed to transform NH ₃ back to H ₂ for use in the DR shaft furnace) data was collected from various sources, as detailed in SI Table S5.24.
Production asset capital costs	Iron and steelmaking furnace capital costs, and the NH ₃ cracker unit cost, have been collected from various sources as detailed in SI Table S5.26.
Emissions boundary and emission factors	Emissions were determined as the sum of scope 1 and 2 emissions (although since all electricity was CO ₂ -free, scope 2 emissions were nil). Upstream scope 3 emissions from raw material extraction, preparation and transportation were excluded. The emissions boundary was drawn around sites, up to the point of crude steel production. For scope 1 emission factors refer to SI Table S5.23.

The major carbon pricing mechanism affecting Ukraine is the EU-ETS, a ‘cap and trade’ market-based mechanism, and its complementary Carbon Border Adjustment Mechanism (CBAM), which imposes a price on carbon within goods imported to the EU. Under anticipated EU accession, all Ukrainian steel production will be subject to the EU-ETS, and on the pathway to EU accession, a similar yet more moderate Ukrainian carbon pricing mechanism is likely to be active (the UA-ETS, see Table 5.3), with exports subject to the EU CBAM.

Table 5.3 Forecasted EU-ETS and UA-ETS policy features. Emission-intensity benchmarks from 2021-2025 are based on the top-10% most efficient facilities with an annual linear benchmark reduction factor of 4.5% from 2026 and 4.6% from 2029. Free allowances reach zero by 2035. Steel classes were slightly modified, adopting ‘primary’ and ‘secondary’ as extensions of the actual ‘hot metal’ and ‘EAF carbon steel’ classifications, respectively.

		Unit	2025	2030	2040	2050	Source
EU-ETS and CBAM	Emission-intensity threshold (primary steel)	t CO ₂ /t steel (scope 1&2)	1.288	1.021	0.638	0.398	European Parliament Research Service (Erbach & Foukalová, 2023); Eurofer (2021)
	Emission-intensity threshold (secondary steel)	t CO ₂ /t steel (scope 1&2)	0.215	0.170	0.106	0.066	
	Reduction factor for free allowances	-	100%	50%	0%	0%	
	Carbon price	USD/t CO ₂	70	100	200	250	OECD (2021b); IEA (2022)
UA-ETS	Reduction factor for free allowances	-	-	75%	0%	0%	Kyiv School of Economics, medium scenario (KSE, 2021)
	Carbon price	USD/t CO ₂	-	75	150	188	

5.3.2 Optimising renewables-based electricity, hydrogen, and ammonia production

This study utilised an integrated energy-production system to optimise the production of three separate renewable-energy derived products: electricity, hydrogen, and ammonia (shown in SI Figure S5.17). In each case, the model considered both the local renewable energy profile and the capital cost of each piece of equipment to determine the system design that minimised the NPV whilst satisfying the product demand. The MILP optimisation was implemented in Python, using the PyPSA module and Gurobi solver. This model was repeated for each product with the requirement of firm power/H₂/NH₃, i.e., continuous supply which could feed the continuous production demands of the steel industry. Green electron production from the solar panels/wind turbines were either directly utilised, stored (in lithium-

ion batteries, in compressed gaseous H₂ tanks, or liquefied NH₃ tanks), or curtailed in every hour over the 8760 hours in the modelled year.

Having determined the minimum cost of the system for energy production, the maximum capacity for energy production of the specific system in every location was then estimated for every 1°x1° grid. Land/sea use reduction factors were applied in acknowledgement that (i) not all areas are suitable for RE infrastructure, nor (ii) can the entire RE potential of an area be solely dedicated to green steel production. These factors are described in Table 5.4.

Table 5.4 Key data inputs to the RE optimisation model.

Data type	Description and source(s)
Solar and wind power potential	Weather data was obtained for the year 2019 from the ERA5 dataset (Hersbach, 2023) and converted into renewable energy profiles using a standard wind turbine curve (considering turbines at 100m altitudes and the Vestas 3 MW model) and the python library PVLlib (using the general Sandia National Labs design for a panel (Holmgren et al., 2018)).
Unit costs for renewable electricity, hydrogen, and ammonia production and storage	To forecast unit costs of emerging renewable electricity and electrolyser technology to 2050, current costs for wind and solar projects in Ukraine were sought (refer to SI Table S5.14) and learning curves from the Oxford Institute of New Economic Thinking applied (Way et al., 2022). Since Ukraine has no existing offshore wind projects, global average floating and fixed capital costs were utilised (Salmon & Bañares-Alcántara, 2022). In oceans at water depths of less than 50m, fixed-bottom wind turbines can be installed; for greater depths up to 1000m, more expensive floating turbines were required; for depths over 1000m, no wind turbines installations were considered. Hydrogen production is based on water electrolysis using low-temperature electrolysers. For the full list of time-variable cost parameters, refer to SI Table S5.15 and Table S5.17. Relatedly, for electrolyser and fuel cell efficiencies, refer to SI Table S5.16.
Land type classification	MODIS5 land classification data (Friedl & Sulla-Menashe, 2019), which uses satellite imagery to determine the current use of the land, of which there are 17 possible land use classifications.
Maximum land consumption for RE infrastructure as fraction of total land availability	For each classification, estimates from literature (Salmon & Bañares-Alcántara, 2022) were applied, which determined the maximum fraction of land that could plausibly be used for renewable energy production. Land was also excluded if it was designated as protected by the UN (Protected Planet, 2023), or if the local slope was greater than 15°. Refer to SI Table S5.13.
Maximum sea consumption for RE infrastructure as fraction of sea availability	For the Black Sea and Azov Sea, an assumption of 50% of the grid area within Ukraine's marine exclusive economic zone was made, considering high-density marine traffic, and marine protected areas (Begun et al., 2012).
Maximum steel sector fraction of maximum RE infrastructure consumption	An assumption of 20% was made for the steel sector's portioned consumption of land, given that pre-war, the Ukrainian steel sector consumed around 20% of final energy consumption. This calculation was based on national consumption of 2.156 million TJ (IEA, 2021d), and energy consumption rates of 23.0 GJ/t consumed by the BF-BOF/OHF route (Metinvest, 2020), and 9.4 GJ/t consumed by the EAF route (Interpipe, 2021).

5.3.3 Establishing scenarios and forecasting steel demand

Two distinct scenarios were developed which reflect the complexity of war and the uncertainty of post-war outcomes, as detailed in Table 5.5. Underlying both scenarios are the assumptions that Ukraine will become a member of the EU, with carbon pricing mechanisms enforced, and the armed conflict is

resolved, thereby reducing investment risk, and creating the fundamental economic conditions for market-competitive green steel.

Table 5.5 Scenario definition.

Parameter	Strong Recovery	Slow Recovery
Land occupation	Full territorial liberation, including the Donbas and Crimea.	Partial liberation of territories; land currently occupied by Russian forces remains under Russian control.
Domestic demand	Strong domestic demand driven by 90% of refugees returning to Ukraine post-war (ref Fig 6 of Kulu et al. (2023)) and complete post-war reconstruction over a 20-year period. Domestic steel consumption rates reach 165 kg/capita by 2050 (from 60 kg/capita during the war).	Weak domestic demand driven by 10% of refugees returning to Ukraine post-war (ref Fig 6 of Kulu et al. (2023)) and partial (80%) post-war reconstruction over a 20-year period. Domestic steel consumption rates reach 150 kg/capita by 2050 (from 60 kg/capita during the war).
Exports	Strong EU export market for green steel and green HBI, given EU membership, and CBAM imposed on extra-regional competitors. Exports reach 16 Mtpa steel equivalents by 2050.	Reasonable EU export market for green steel and green HBI, given eventual EU membership, and CBAM imposed on extra-regional competitors. Exports reach 11 Mtpa steel equivalents by 2050.
Trade routes	All sea routes open and rail de-bottlenecked.	No access to Azov Sea ports, but rail de-bottlenecked.
EU accession	Rapid EU accession (by 2030).	Slow EU accession (by 2040).
Carbon policies	EU-ETS adopted.	Medium UA-ETS implemented in 2030, and CBAM is imposed on EU/UK exports. EU-ETS adopted by 2040.
DR-grade ore availability	DR-grade ore supply expands (in response to R&D and investments in beneficiation and pelletisation capacity), reaching 23.7 Mtpa in 2050 (34% of total ore products, satisfying 80% of total production demand).	Stagnated DR-grade ore supply (with minimal R&D and investments in beneficiation and pelletisation capacity), reaching 11.9 Mtpa in 2050 (17% of total ore products, satisfying 64% of total production demand).

Dynamic material flow analysis (MFA) was utilised to understand the historical inflows, outflows, and in-use stocks of steel in Ukraine, facilitating projections of post-consumer steel demand and scrap supply out to 2050. Historical steel consumption allocation across the key product categories (transportation, machinery, construction and appliances/packaging) were estimated using input-output (I-O) tables from the available data years: 1972 (Gillula, 1983), 1990-1995 (Aptekar & Amosha, 2005), and 2013-2020 (State Statistics Service of Ukraine, 1990-2021). Following work by S Pauliuk et al. (2013), saturation levels for mature steel stocks were determined to be 13±2 tonnes/capita, and a normally distributed lifetime assumed with standard deviation of 0.3 to the mean. Scrap steel availability was determined using a 90% recycling rate (worldsteel, 2023) of post-consumer steel outflows.

Domestic steel demand was calculated as the sum of population-based consumption and reconstruction-related needs. For population-based steel consumption, annual per capita consumption rates were multiplied by the projected population, as specified in Table 5.5 for each scenario. For reconstruction-related needs, estimates of the direct damage to Ukraine's buildings and infrastructure in the first 12-months of the war has been valued at \$134.7bn (World Bank Group, 2023) which will cause a total demand boost of \$12.63bn per year in Ukraine's construction industry over a reconstruction period of 10 years (refer to SI Table S5.11). This will generate \$2.77bn of additional steel

demand per year, equivalent to 15.5% of the 2021 annual output, or 3.32 Mtpa steel. It can be reasonably assumed that damage will increase at least two-fold in the subsequent hostilities from February 2023 onwards, totalling 66.4 Mt steel for post-war reconstruction needs over a period of 20 years. Post-war reconstruction will significantly boost demand for steel products, spanning infrastructure repair, defence requisites, and economic revival, and it is in Ukraine's economic interest to meet this surge in steel demand via domestic production.

Export demand for green HBI and green steel products were informed largely by historical trade patterns, and the landscape of existing steelmaking technologies within importing nations. Exports were distributed over the 13 EU member states and the UK. To safeguard supplier diversity, exports could not exceed 35% of any nation's projected demand (given by Bataille et al. (2021)) according to the scenario with 2.2Bt of steel demand in 2050). HBI could be produced using BF-grade or DR-grade ore, and the demand of each sub-product was a function of the relative existing capacities of BF-BOF (supporting BF-grade HBI via the DRI-melt-BOF route) and EAF (supporting DR-grade HBI via the DRI-EAF route) plants in each importing country. The fundamental assumption was the maintenance of an export-oriented industry in Ukraine. Over the past decade approximately 75% of the produced steel has been directed towards exports and the steel sector has generated around 25% of the nation's commodity exports, with \$16bn worth of exports in 2021 alone (State Statistics Service of Ukraine, 2000-2021). Pre-invasion, Ukraine ranked 14th among steel-producing countries, with a total output of 21.4 Mt (million tonnes) of crude steel, and 15.7 Mt exported (worldsteel, 2021b). To note, Ukrainian steel products have been historically subjected to a vast variety of anti-dumping measures by countless foreign trade partners (refer to SI Table S3.3). A green steel transition, thus, is vital for this sector to survive growing de-carbonisation pressures in the country's key export markets.

5.3.4 Deriving economic multipliers from input-output analysis

I-O analyses utilise a systems approach to the economy, stressing inter-industrial or sectorial interdependence whereby the output of one sector is often the input of another (Leontief, 1966). This study employs macro-economic analysis to (i) examine the impact of the Ukrainian steel industry on production, income, and growth and (ii) model the long-term effects of post-war reconstruction on domestic steel demand and on the wider economy. Through a detailed disaggregation of economic activities, Leontief inverse matrices were developed, providing quantitative transaction relationships between industrial components of a given economic system (Leontief, 2008). I-O multiplier analysis was selected as the most analytically rigorous approach to regional modelling in comparison with the two alternatives – the Keynesian income multiplier and economic base models (McCann, 2013). Three core assumptions were applied: proportionality (i.e. demand for intermediate inputs is a linear function of output), constant returns, and no substitution between different inputs or factors of production (Munroe & Biles, 2005). Following guidance from key practitioners (Eurostat, 2008; UK Office for National Statistics, 2022) and based on data from the Ukraine State Statistics Service (1990-2021), an economic analysis of the historical coal-based steel sector was conducted for 2014 and 2021. In addition, the macroeconomic impact of the optimised future green steel sector was modelled for national output, income, and gross value added (GVA) patterns. For comparison, the economic impact of the

same magnitude of steel production under traditional coal-based steel scenarios was assessed and modelled using the latest pre-war output multipliers.

5.4 Results and Discussion

5.4.1 Green sectorial growth is underpinned by strong regional demand and product market competitiveness



Figure 5.2 Ukraine steel demand projections, inclusive of exports, domestic consumption, and additional reconstruction needs, for the (a) Strong Recovery scenario, and (b) Slow Recovery scenario, respectively. Exports are a combination of green HBI and green steel, expressed as steel equivalents (given 0.9t HBI/t steel for 14% scrap charging during steelmaking).

Trade links with regions governed by strong climate policies drive progress in decarbonising export-oriented steel sectors. Reconstruction efforts will initially drive steel demand, but insufficient alone to drive sustainable industry growth. In the *Strong Recovery* scenario, EU accession is achieved by 2030, resulting in immediate realisation of ‘demand-pull’ for green steel and HBI products from export markets; the steel export ratio was estimated to be 58% in 2030, expanding to 77% by 2050 (on par with the pre-war ratio, as shown in Figure 5.2). It is essential to take advantage of two important export markets:

green steel, and green HBI. Whilst green steel offers greater export revenue prospects, HBI will be an extremely valuable negotiation tool for trade partnerships. Unlike the traditional integrated BF-BOF production route, ironmaking and steelmaking can be separated in the DRI-EAF route through the transport of HBI. Traditional large EU steel manufacturing economies, e.g., Germany and Spain, will be more open to benefit-sharing agreements, whereby Ukraine carries out ironmaking, and they maintain steelmaking capacity and value-adding downstream processes. This approach safeguards jobs for both parties, whilst improving overall market competitiveness. Ukraine would still obtain significant export revenues from green HBI; if the EAF is charged with 100% DRI, HBI costs would represent about 75% of the cost of steel. The maximum total export quantity for any scenario is 17 Mtpa of steel equivalents, representing a reasonable 11% of the total demand from EU-27 and the UK in 2050. Moreover, long-term trade partnerships with numerous countries and modest export expansion plans support investment risk reduction and green steel sectorial growth.

Market competitiveness is necessary to establish and sustain new trade partnerships. In the context of EU accession, Ukraine's steel and HBI exports will shift away from traditional North African and Middle Eastern markets, and towards EU and UK markets (as shown in SI Figures S5.7-S5.9). Although pre-war Ukraine exported 15 Mtpa steel products, only 2.5 Mtpa was directed to European nations (Eurofer, 2022). Exports are anticipated to be directed to EU and UK neighbours as they have clear carbon policies including border adjustment mechanisms. To secure a reasonable share of Europe's green steel market, a required levelised cost of steel (LCOS) less than or equal to \$500-586/t has been estimated (Lopez et al., 2022). Fortunately, Ukraine's green LCOS range in ideal locations has been calculated in this study as \$440-600/t. At the lower end, H₂-DRI-EAF production is powered by firm electricity from hydro or nuclear power where costs are minimised due to the fully depreciated assets of these mature energy projects (although for new builds, these energy resources may prove very expensive). At the pricier end, co-located H₂-DRI-EAF production will cost around \$587/t steel, based on cost-competitive continuous supply of electricity (\$64/MWh) and green hydrogen (\$3.31/kg H₂) using new-build onshore hybrid solar and wind power (see Figure 5.3). About 75% of the costs of steelmaking occur up to the point of iron production; the levelised cost of green HBI is estimated at \$440/t, and with cheaper firm electricity of \$20/MWh costs reduce to \$290/t. This is competitive with green HBI costs estimated for other ore-producing regions, e.g. \$395/t in South Africa (Trollip et al., 2022), especially considering the reduced transportation costs. Tapping into high quality renewables is essential for HBI and steel production cost reduction and export market retention.

5.4.2 Multiple zero-emissions energy sources support the transition

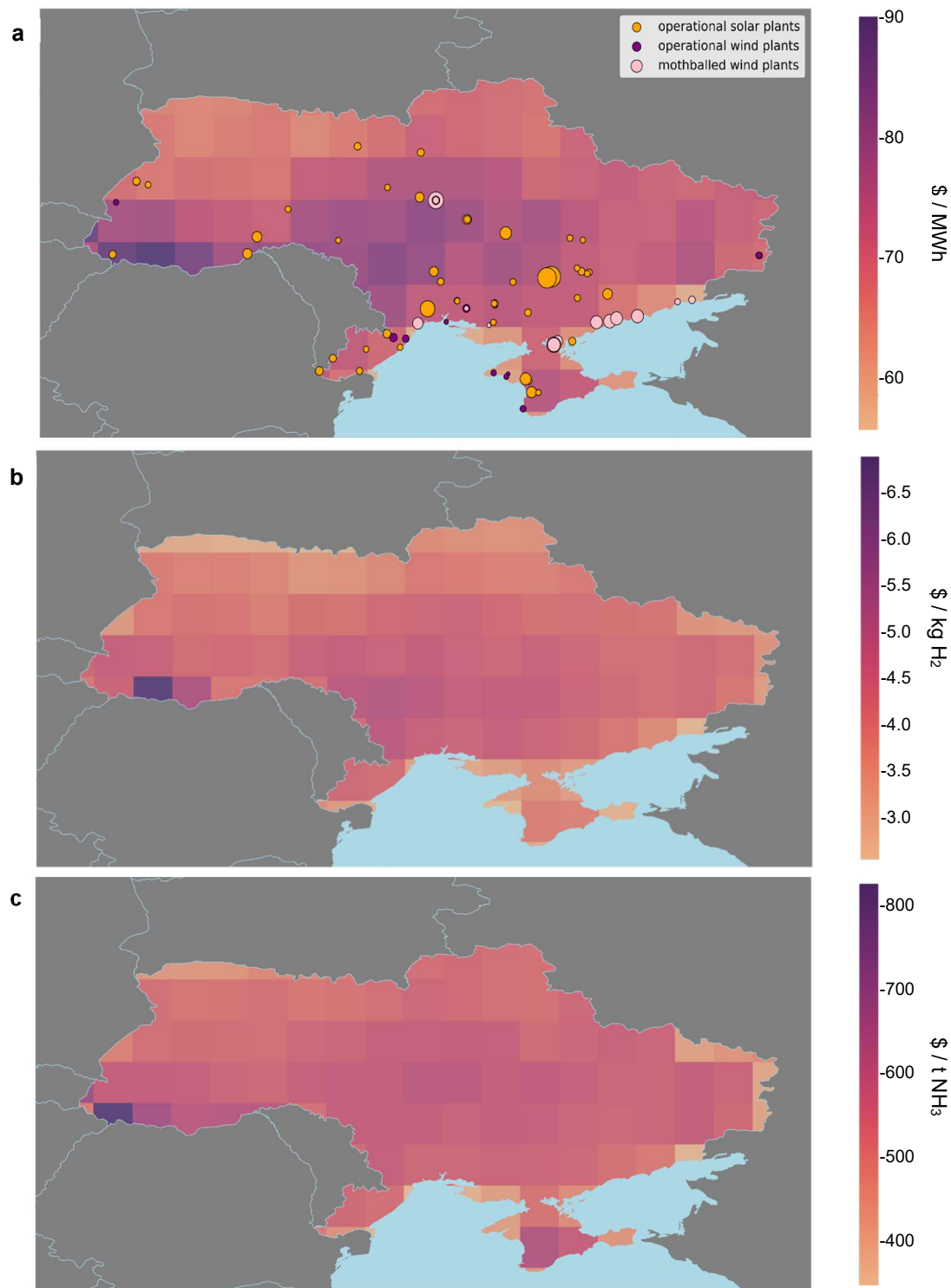


Figure 5.3 Cost-minimised results of onshore hybrid solar and wind plant energy products installed in 2050 - (a) Levelised cost of firm electricity (in USD/MWh), plotted with existing solar and wind installations (markers sized according to capacity). (b) Levelised cost of continually supplied hydrogen (in USD/t H₂). (c) Levelised cost of continually supplied ammonia (in USD/t NH₃).

Significant temporal and spatial variability in renewable potential exists across the region. The LCOE for firm power from onshore hybrid solar and wind energy is quite high, varying from \$86-161/MWh in 2030, \$70-117/MWh in 2040, and \$58-91/MWh in 2050 (as shown in Figure 5.3a). Despite the strength of wind resources in Ukraine (in 2019, the average hourly power capacity for wind was 0.32 and for solar 0.14), the high expense of wind turbines in comparison to solar panels favours the latter. Solar capacity as a portion of total renewable energy capacity was on average 68% in 2030, increasing to 78% in 2050. Daily and seasonal troughs in solar power are somewhat balanced by peaks in wind power, with reduced intermittency and increased wind speeds observed in winter months when solar power is reduced. The LCOH is similarly un-exceptional: results vary from \$3.96-13.76/kg H₂ in 2030, \$3.19-9.45/kg H₂ in 2040, and \$2.65-6.91/kg H₂ in 2050 (as shown in Figure 5.3b), which for even the best locations is above the EU's goal of electrolytic hydrogen costs below \$2.2/kg H₂ (€2/kg) (EurActiv, 2021). The LCOA varies from \$450-1300/t NH₃ in 2030, \$389-1027/t NH₃ in 2040, and \$346-829/t NH₃ in 2050 (as shown in Figure 5.3c), with the upper quartile in 2040 and 2050 being competitive with the conventional emissions-intensive natural gas-based production method of \$300-550/t NH₃ (IEA, 2020c). Ideal locations for onshore green power and fuel production are in far Southern, Eastern, Northern and North-western regions, which strike a balance between reliability (i.e., minimal intermittency) and intensity (i.e., power output) of solar and wind resources.

Utilising hydropower and nuclear power can reduce energy costs, but capacity is highly constrained. For firm electricity delivered at \$20/MWh, the LCOH is outstandingly viable at \$1.23, \$1.14 and \$1.06/kg H₂ in 2030, 2040 and 2050, respectively. This cost-competitiveness is extended to ammonia, costing \$321, \$305, and \$291/t NH₃ in 2030, 2040 and 2050, respectively. However, under HPP constraints, the steel sector may consume 19 TWh of electricity annually which can power 5 Mtpa of green H₂-DRI-EAF steel production, and under NPP constraints, the maximum consumption is 3.2 TWh annually or 1 Mtpa of green H₂-DRI-EAF steel. In addition, whilst solar and wind projects offer rapid project development and construction times (a recent 240 MW solar farm in Ukraine took just 8 months for construction (DTEK, 2019), and a 114 MW wind farm took 1.5 years even during the war (DTEK, 2023)), nuclear projects require decades from final investment decision to operation with the construction period alone being about 9 years (World Nuclear Association, 2020). Hence, whilst mature CO₂-free energy infrastructure has a role to play, energy system expansion relies on solar and wind.

Renewable energy potential is high and aligns well with literature. Nation-wide, the onshore solar and wind power potential in 2030 summed to 2182 TWh (maximum 436 TWh allocated to the steel sector), calculated with hourly wind speed at over 100 locations. This estimate is 70% greater than the estimate by the Ukrainian Institute of Renewable Energy (Ukrainian Institute of Renewable Energy, 2020). At the same time, the estimated green H₂ potential of 40.8 Mtpa (maximum 8.3 Mtpa allocated to steel sector) aligns closely with the Ukrainian Institute of Renewable Energy's wind-to-H₂ assessment (Kudria et al., 2021). The combined sea capacity for energy production was 205 gigawatts (GW), producing 288 TWh in 2050, equivalent to 54% of combined land capacity, roughly aligning with World Bank estimates (World Bank Group, 2020) of 250 GW. In this study, it is estimated that Ukraine comprises 12.7% of EU land which is available and suitable for installation of renewable energy infrastructure, preceded only by Spain (14.8%) and France (13.2%). Ukraine could be a significant contributor to EU energy security through export of energy-intensive manufactured products.

5.4.3 The sectorial transition is supported by well-timed investments, geographical and energy source diversity, and carbon pricing

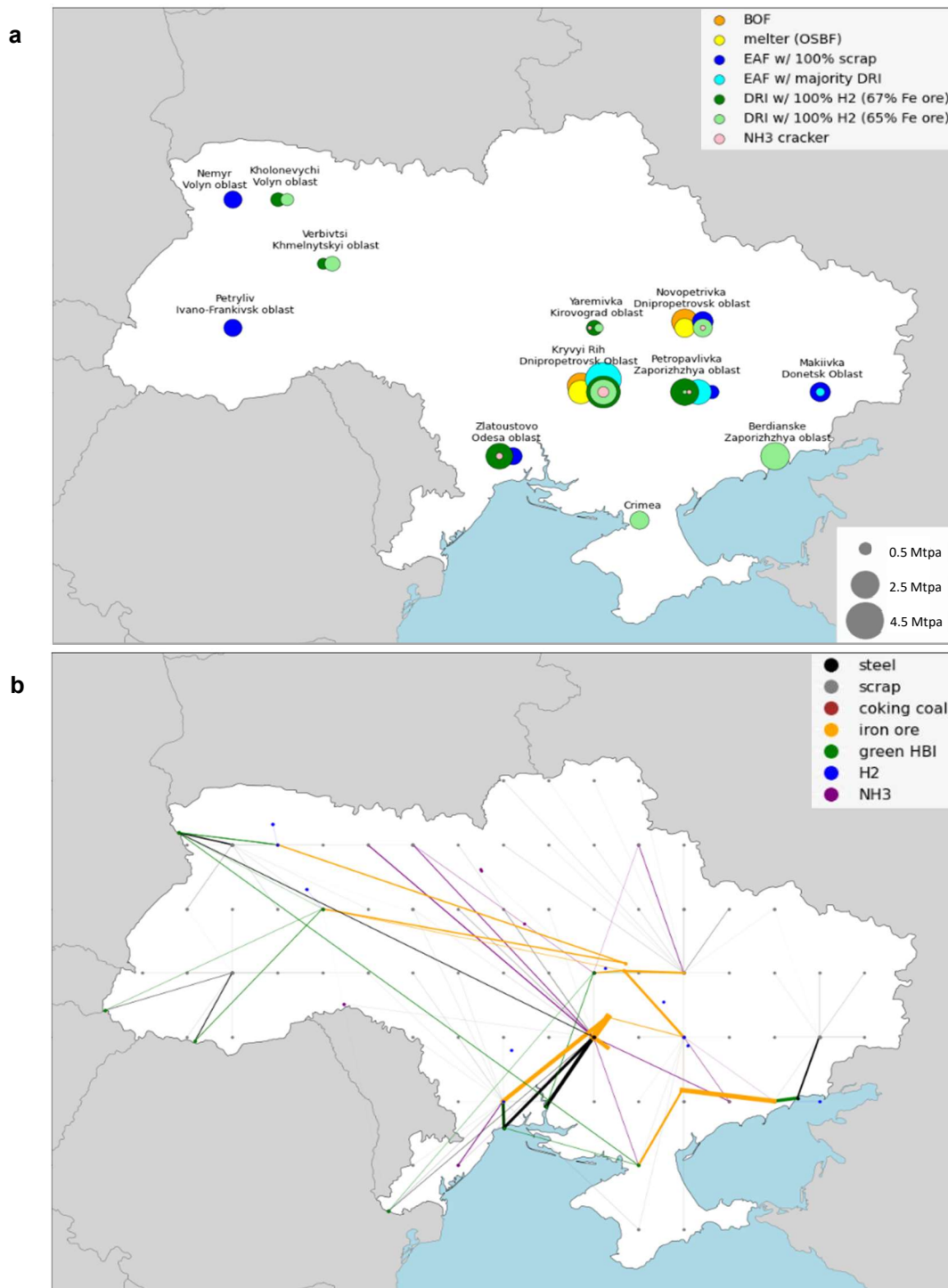


Figure 5.4 Optimised steel supply chains in 2050 under the Strong Recovery scenario: (a) capacity of iron and steel production assets (colour indicates technology and marker diameter indicates plant capacity), and (b) domestic supply chain flows (straight-line distances shown, line thickness indicates trade volume) including transportation of green steel exports to ports. See SI Figures S5.12 and S5.13 for 2030 and 2040 results, respectively.

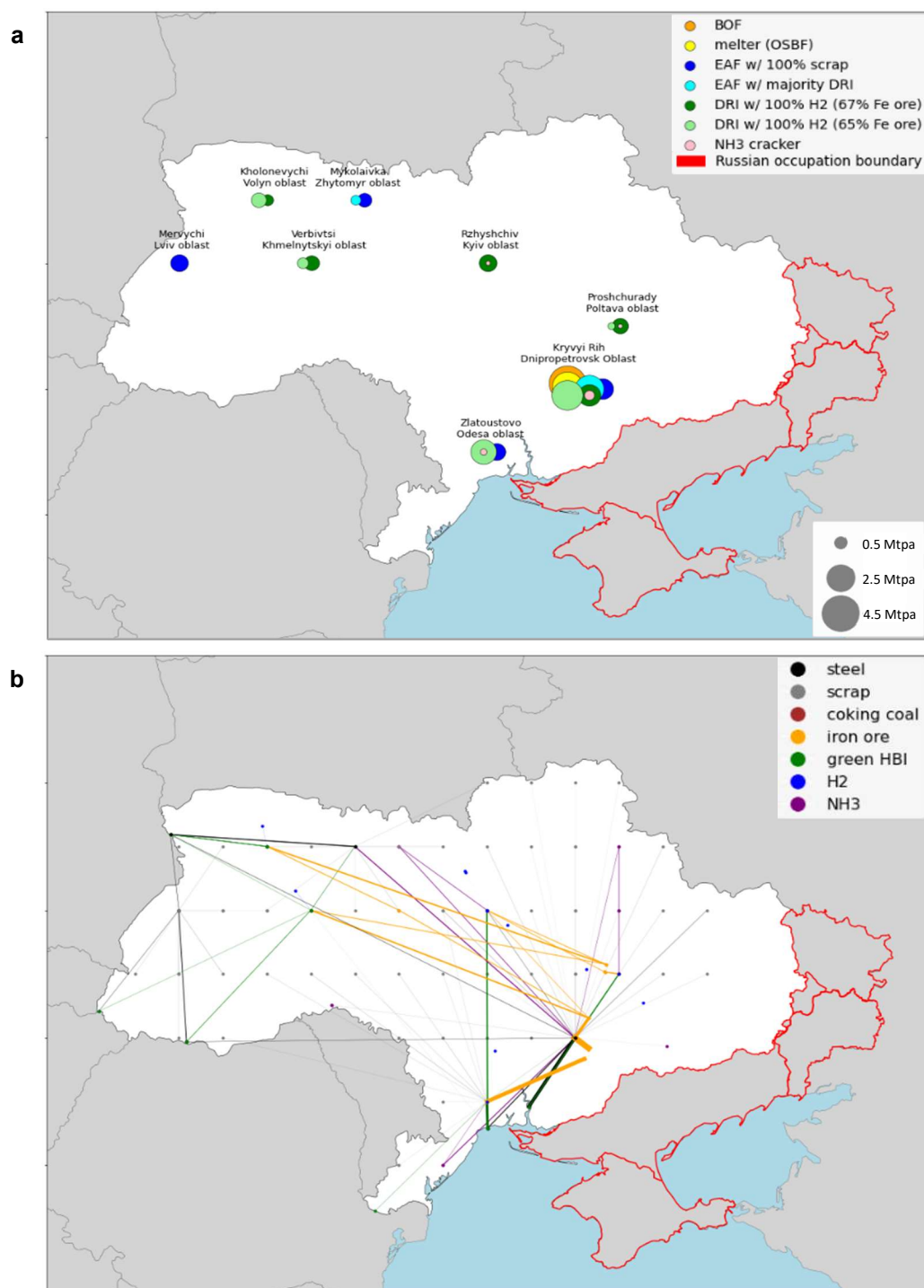


Figure 5.5 Optimised steel supply chains in 2050 under the Slow Recovery scenario: (a) capacity of iron and steel production assets (colour indicates technology and marker diameter indicates plant capacity), and (b) domestic supply chain flows (straight-line distances shown, line thickness indicates trade volume) including transportation of green steel exports to ports. The geospatial data for Russian-occupied regions are given by Deep State UA (2023), accurate as of April 2023. See SI Figures S5.14 and S5.15 for 2030 and 2040 results, respectively.

A gradual, integrated sectorial plan to achieve near-zero emissions in 2050 supports successful transitions: 2030 is a critical near-term milestone. Ukraine's existing coal-based steel plants are of significant capacity; nevertheless, Soviet-era assets are aged and carry little inertia, making green steel

project investments more convincing. By 2030, 43 individual furnaces of operating/mothballed status will require an investment decision to continue/restart operations or entire retirement (19 x BF, 13 x BOF, 8 x OHF and 3 x EAF). In 2030, the average BF age will be 61 years, and the average economic lifetime remaining on the latest reline will be 6 years (GEM, 2023a), therefore, few assets will face substantial debt for early retirement. In addition to the forthcoming carbon taxation of steel imports into the EU, UK, and other G7 nations, the age of BF assets in Ukraine, significantly greater than the global average of 25 years (Swalec & Grigsby-Schulte, 2023), supports the green investment case. For the *Strong Recovery* scenario, in 2030, just 12% of existing blast furnace capacity continues operation, totalling 3.5 Mtpa iron capacity across three plants. About one-third of basic oxygen furnaces continue to be used to facilitate integrated BF-BOF production, totalling 5.1 Mtpa. To meet the production gap, 10.8 Mtpa of additional DRI capacity and 7.2 Mtpa of additional EAF capacity (on top of the existing 3.8 Mtpa of existing EAF capacity) will need to be installed. By 2050 (as shown in Figure 5.4), across five brownfield (i.e. previous steelmaking site) and seven greenfield (i.e. new steelmaking site) locations, ironmaking capacity will be completely H₂-based, with steelmaking being distributed across the following processes: 42% scrap-based EAF, 37% DRI-charged EAF, and 22% melter-BOF. With less than three decades remaining to 2050, early investments in low and near-zero emissions production technology are vital to support smooth transitions.

Greenfield sites offer new opportunities to take advantage of high-quality renewables. The utility of green NH₃ and green HBI trade increases the geographical diversity of plant locations. Kryvyi Rih remains a dominant steelmaking region, adjacent to the nation's largest iron ore basin and near Black Sea ports, with cheaper NH₃ transported from northern locations. In the balance of optimality and feasibility, iron and steel plants are concentrated in central-eastern and north-western regions. The need for greenfield projects in the Western and Central parts of the country will be especially high for Ukraine, if Russian-occupied territories, and the existing steel plants contained there, remain inaccessible (as shown in Figure 5.5). In the *Slow Recovery* scenario, despite reduced steel demand, the lack of access to existing assets will drive new furnace investment. In 2030, 6.9 Mtpa of DRI and 4.9 Mtpa of EAF capacity would need to be installed across six greenfield sites and one brownfield. In 2040, further investments will total 2.1 Mtpa of DRI, 1.7 Mtpa of OSBF, and 2.2 Mtpa of EAF capacity. By 2050, any remaining BF capacity will be retired, and the production gap met by new DRI and melters (OSBFs) to be combined with existing BOF capacity for steelmaking with lower quality HBI. Construction in north-western regions furthest from the frontlines could be prioritised, where plants benefit from cheap local renewables and proximity to rail border crossings.

The transition is supported by mature CO₂-free energy sources (nuclear and hydropower), rather than natural gas. Although considered a transition fuel, natural gas is nonetheless a CO₂-producing fossil fuel, with carbon prices to be imposed on it. By 2050, domestic natural gas reserves will also likely be depleted, so it is logical for the sector to refrain from gas dependency, aligning with the recent REPowerEU policy (European Union, 2022b) that intends to reduce reliance on Russian gas imports. The immediate period, however, from now until 2030, may benefit from H₂/NG blends, as the price reductions of nascent electrolysis technology is accrued. Cost, rather than supply constraints, is the key

determinant of NG redundancy: even without a price on carbon, the NG-DRI-EAF production costs come to \$480/t steel based on NG supply at \$25/MWh, more expensive than the H₂-DRI-EAF production route with continuous electricity supply at \$20/MWh, coming to \$430/t steel. For the *Strong Recovery* scenario of 2030, all electrical energy, and the majority (69%) of chemical energy is delivered by onshore solar and wind, whilst the chemical energy gap is filled by nuclear (19%), offshore wind (11%) and hydropower (3%). Moving forward, the expansive capacity of solar and wind is relied on to energise the increase in green steel demand. Tapping into cheap renewables, either locally via electricity or H₂ supply, or regionally via NH₃ supply, is critical to competitive green steel production.

5.4.4 Demand-driven change multiplies cost-effectiveness of green steel investments

Multibillion-dollar industrial investments require concerted financial support. Simultaneously to rebuild the 22 Mt Ukrainian steel industry and transition to near zero-emissions by 2050, the necessary infrastructure investments surmount to \$45.9 billion for renewable energy, \$6.6 billion for energy storage, and \$9.5 billion for furnaces (given full liberation of Ukrainian territory). Furthermore, the export-oriented industry needs highly efficient railway and sea passage trade routes to attain market competitiveness. Transport is more efficient via shipping vessels; whilst railway infrastructure would need major revitalisation to achieve time and cost efficiencies, including matching Ukraine's railway gauge with that of Europe's, and upgrading capacity to support 9.5 Mtpa of HBI/steel exports. Pipelines must also be installed to deliver 2.6 Mtpa of liquefied NH₃ by 2030, and ports upgraded to manage 6.3 Mtpa of green HBI/steel exports. Ore beneficiation and pelletising capacity must also be bolstered to deliver 9.6 Mtpa of DR-grade ore. Systemic industrial change of this magnitude requires immense mobilisation of capital, for which financial support in the form of both carbon prices and clean technology incentives are needed. The EU-ETS and CBAM policies are crucial for carbon pricing, but Ukraine also requires significant foreign financial support to drive its industrial transformation and attract global investments.

At the same time, steel industry investments will cause ripple effects across the economy. In 2021, for every \$1 invested in the basic metals industry, an additional \$3.28 was generated elsewhere in the economy through indirect and induced effects (based on the Type II multiplier, see SI Table S5.10). A comparative macroeconomic assessment was undertaken of the: (i) emissions-intensive coal-based steel sector, and (ii) transitioning green steel sector associated with the *Strong Recovery* scenario. Results show that a green steel sector will benefit the economy with stronger supply chain linkages, income generation, and gross value-added under most scenarios. For the 2030 green steel sector over its 20-year project lifetime, the Ukrainian economy is forecast to generate \$446bn of steel sector-driven output, \$88bn of income, and \$269bn of GVA. The corresponding coal-based steel sector would generate less income (\$81bn) and far less GVA (\$192bn) (refer to SI Figure S5.16). I-O analysis of future green steel production is indicative, for it is based on historical compositions of the traditional electricity and chemical industries – growing renewables shares in the electricity sector and electrolytic processes for H₂ and NH₃ production will change how these sectors interact with the economy, and perhaps even bolster it. Nevertheless, a strong correlation between the proposed green steel sector

and economic growth is determined. The structural transformation of the mining and metals industries into a value-adding green steel sector will return far-reaching economic benefits, stimulating employment, supply chain expenditure, and sustainable export revenues.

5.5 Conclusions

This study explores tensions between optimism and realism to assess possibilities for Ukraine to build back greener in its steel sector. Transitioning from a coal-dependent to renewables-dependent steel industry is feasible given clear climate policies, strong regional trade links, and access to capital. Multiple factors favour Ukraine's green steel potential: valuable iron ore resources, reasonable solar irradiation and wind speeds, large land mass, high-flowing rivers to support cheap hydropower, uranium resources to support nuclear power, low wages, and proximity to EU green steel markets via ports and railways. Prospective EU accession makes steel decarbonisation non-negotiable, whilst opening critical green export markets. Moreover, whilst the core capital investment needed for Ukraine's green steel transition amounts to \$62bn over a 20-year period (excluding the required connectivity upgrades), a green steel sector alone will generate \$77bn worth of additional GVA more than the corresponding coal-based steel sector, *ceteris paribus*.

A mixed energy portfolio will balance the intermittency of renewables across time and space: solar, wind (onshore and offshore), hydro, and nuclear, among other sources, can contribute to the integrated fossil-free energy system. There are multiple pathways to near-zero emission by 2050, and no single technological solution is ideal. The results shown here encompass H₂-DRI-EAF, H₂-DRI-melter-BOF, and scrap-based production routes, but emerging solutions like direct iron ore electrolysis may also play a role in the EAF technology mix once they reach maturity. Greenfield sites take advantage of the cheapest renewables available. Although brownfield sites benefit from established transport links and local skilled labour pools, these are diminished in a post-war context, where significant infrastructure destruction has occurred, and communities dislocated. Managing risks associated with fossil fuel asset 'lock-in' (i.e., emission inertia caused by physical and economic constraints) and stranded assets (i.e., infrastructure that becomes redundant before the end of its anticipated economic lifetime) are critical in the steel sector's decarbonisation pathway, given the industry's capital-intensity and long amortisation periods.

The results transcend the Ukrainian context (21.4 Mt steel produced, 15.7 Mt exported in 2021) to other iron ore-producing nations with export-oriented steel industries: for example, Brazil (36.2 Mt steel produced, 11.5 Mt exported) and Vietnam (23.0 Mt steel produced, 11.2 Mt exported) (World Steel Association, 2022). In future work, the supply chain optimisation model can be modified for any geographical context and spatial scope. Significant efforts were made to utilise Ukraine-specific resource constraints, geospatial data, renewable energy infrastructure costs, commodity prices, carbon prices, domestic steel demand and green iron/steel export projections, which must be modified for each specific case. Flexibility within the integrated energy system could be explored further, for example, regarding the use of dispatchable nuclear/hydro in lieu of battery/CGH₂ storage for renewables. To share some preliminary insights, it was deduced that flexible H₂-DRI-EAF production with up to 25%

dispatchable power allowance at \$25/MWh reduced the LCOS by 27%. Finally, this work did not address environmental and social issues beyond climate change; a holistic sustainability impact assessment framework should be developed for the green steel industry.

Chapter 6. Discussion and Conclusions

6.1 Research summary

Through a systems engineering perspective of technology-led changes, this thesis tested the hypothesis that *industrial relocation will support industrial decarbonisation*, on the quest to explore the new steel map. Focussing on ore-based steelmaking, novel renewables-based steel supply chains were explored under a geospatial explicit supply chain optimisation framework, and the following research questions addressed:

- Globally, what locations are favourable for integrated green H₂-based steel production, considering the relative attractiveness of localised inputs: renewable energy, iron ore, scrap, and wages? What new green steel markets may emerge with competitive green steel production costs, and the potential to scale-up? [Chapter 3]
- Regionally, can transnational alliances be employed to shift traditional roles in the iron and steel value chain and increase green steel market potential? Considering green H₂-based steel production, what are the energetic and economic benefits of co-locating hydrogen, iron and/or steel production with high quality renewables and iron ore deposits? Can green HBI trade corridors support efficient and distributed green steel production? [Chapter 4]
- Nationally, what technology investments are required when, and where, for the industrial transformation to near zero-emissions production? What transitional energy sources and technologies will emerge as influential, especially when considering iron ore quality constraints and the availability of near zero-emissions energy sources, including mature hydropower and nuclear power? To what extent does existing fossil-based asset inertia affect the green steel project investment case? How can regional trade links, strong demand signals for green steel, and carbon policies, support sectorial decarbonisation? [Chapter 5]

To answer these questions, three major research projects were carried out which offered original theoretical models concerning renewables-based steel production and trade. The thesis commenced with a global assessment of green H₂-based steel market competitiveness using a facility-level optimisation model with high temporal resolution (Chapter 3). The comparative analysis concerned greenfield sites powered by islanded solar and wind energy, and the simplest supply chain in which green H₂, iron and steel production were integrated and co-located with iron ore deposits. Cost-minimised steel production was determined for 17 important iron ore producing countries covering 44 distinct regions, which were then fed into a machine learning model alongside corresponding statistical renewable energy data to increase the spatial resolution to over 300 global iron ore deposits. A supplemental analysis of grid-powered green- H₂ based steel production was carried out to reveal the

economic effects of regionally unique grid emission factors, industrial tariffs, and anticipated carbon prices, and consequently explore the importance of islanded energy systems in enabling energy independency from fossil-dependent electricity networks.

Next, a binational supply chain analysis was undertaken, using the Australia-Japan strategic partnership as a case study (Chapter 4). Technological focus was maintained on the green H₂-based DRI-EAF route, powered using islanded hybrid onshore solar and wind energy. A supply chain simulation model was developed, covering three unique supply chain configurations: (i) iron ore and H₂ exports, (ii) HBI and H₂ exports, or (iii) steel exports, from Australia to Japan. A total of 12 cases were assessed, with variance in supply chain configuration, model year (2030, 2040 or 2050), and H₂ carrier (NH₃ or LH₂), and compared against the key metrics of total energy consumption and production costs. By expanding the steel production boundary from 1 Mtpa at facility-level (as in Chapter 3), to 40 Mtpa at regional-level, the system feasibility could be assessed in terms of finite land and water resources.

Finally, a deep dive into Ukraine's post-war green steel opportunity was undertaken using an iron and steel production and trade optimisation model (Chapter 5). This case study enabled a unique geopolitical framing in the context of EU accession and long-term carbon pricing signals from the EU-ETS and supporting CBAM. At national-level, detailed characterisation of the existing asset fleet was carried out and asset inertia between the modelled years of 2030, 2040 and 2050 applied. A larger breadth of energy sources was assessed, covering fossil fuels (metallurgical coal and natural gas) and both mature and nascent zero-emissions sources (onshore solar and wind, offshore wind, hydro and nuclear). Simultaneously, a range of steel production routes were modelled, including the existing BF-BOF, scrap-based EAF, and NG-DRI-EAF routes, and the emerging H₂-DRI-EAF and H₂-DRI-melter-BOF routes. Moreover, dynamic material flow and trade pattern analysis was performed to forecast post-war steel demand and scrap availability. Rather than the key metric being LCOS, this study valorised a wider range of economic indicators, including induced and indirect spending effects.

The three original research chapters employed three distinct methods for renewable energy cost estimation, with consequent variance in LCOH and LCOS results. In Chapter 3, Renewables Ninja solar and wind power potential profiles were inputted into the optimisation model, with the dataset covering 8760 hours per year, and the 5 years from 2015-2019 modelled. In Chapter 4, Homer Pro microgrid software was utilised which effectively outsourced energy system modelling, simply requiring user inputs for economic and operational parameters and location selection. Finally, in Chapter 5, raw climatic data from the ERA5 dataset covering 8760 hours from the year 2019 was utilised which required the most sophisticated energy system modelling. The final method was decidedly the most accurate as the energy system modelling was internalised, although repetition over a range of historical data years is advised to reduce the impact of interannual variability. It is stressed that the economic metrics presented in this work are indicative, and highly sensitive to the economic input parameters and renewable energy profiles.

6.2 Key learnings and contributions

A few overarching conceptual learnings can be derived from this industrial decarbonisation research. Most significantly, the thesis has proven that it is often energetically and economically rational to reconfigure iron and steel supply chains to tap into high quality renewables and iron ore, and therefore take advantage of novel H₂ and HBI and trade paradigms. Efficient operations are essential to reduce upfront capital and ongoing operational costs, the extent of land acquisitions, and the demand for critical minerals (required for solar panels, wind turbines, electrolyzers, and batteries), and thereby increase the feasibility of scaling up. Globally, there is an unequal distribution of natural (iron ore, energy, land), recycled (scrap), human, and capital resources; strategic co-location of energy-intensive production processes with these resources will underpin the investment case for green steel projects. In addition, the sector must collaborate with suppliers for the industrial paradigm shift; the success of steel decarbonisation depends on the easing of supply chain blockages, especially improving iron ore quality through innovation in beneficiation processes, and scrap quality through innovation in contaminant removal technology. Finally, strategic transnational trade links, policy-led financial levers (i.e., carbon prices or incentive schemes) and market willingness to pay a green premium, underpin the green steel project investment case. The studies have offered new business models to industry, and the impetus to develop effective climate and trade policies for policymakers.

More specific takeaways can be drawn from each key research chapter. In *Chapter 3*, the global survey of green H₂-based steel production costs using islanded renewable energy systems demonstrated that regions surrounding the Tropic of Capricorn and Cancer possess strong solar resources, with good supplementary wind resources, to reliably power production processes. The most influential factors for cost-competitive production were (in descending order): solar and wind power potential and continuity (daily and seasonal reliability), iron ore quality, scrap availability and price, then wages. The model's high temporal resolution (hourly) and repetition using five historical renewable energy years revealed energy-production dependencies: whilst hydrogen production flexibility was essential, due to the continuous production requirements of DRI, few gains were observed by operating the EAF in a flexible batch mode. Hence, driving down production costs of renewable electricity and green H₂ were the most integral components of cost-optimisation. The research showed that green H₂-DRI-EAF steel production may be cost-competitive with coal-powered BF-BOF production in favourable locations in the next decade even without carbon prices, but this relationship relies on the continued decline in costs of nascent renewable energy and electrolysis units, and comparatively high metallurgical coal prices.

In *Chapter 4*, the results showed that importing green iron and steel from regions with abundant renewables, into regions characterised by renewable deficits (i.e., lack of suitable land availability, and/or exposure to reliable and strong energy sources) for subsequent processing into finished steel products, will support green steel market competitiveness and system scale-up feasibility. The distributive trade paradigm is incredibly useful: by dislocating iron and steel production, the energy-intensive iron ore reduction process can be carried out where iron ore and renewable energy resources are abundant, and the value-adding steel production processes which feed into downstream product

manufacture can remain in the traditional steelmaking region. Whilst complete iron and steel supply chain relocation pertains significant geopolitical risks, green HBI trade offers a powerful negotiation tool for strategic transnational alliances. The research provided the impetus for typically extractive economies (i.e., iron ore and coal exporters) to transform into renewables-based manufacturing economies (i.e., green iron and steel exporters). The Australia-Japan case study is relevant for several other strategic alliances where an iron ore exporter with renewables affinity can be matched to a traditional steel producer (and/or steel demand market) with iron ore and renewables deficits. Whilst Australia produced 54% of global exports of iron ore (by value) in 2021, it was followed by Brazil (21%), Canada (5%), South Africa (4%), Ukraine (3%), and Sweden (2%) (Observatory of Economic Complexity (OEC), 2023), which are all eligible producers of green iron and steel. On the receiving end, the largest global importers of iron ore were China (66% by value), Japan (7%), South Korea (5%), Taiwan (2%), Netherlands (2%), and Germany (2%) (OEC, 2023) which could all benefit from green iron and/or steel imports. Intra-regional trade networks may prove advantageous due to proximity, for example, an Asia-Pacific network with Australia exporting to China/Japan/South Korea/Taiwan, or a European network with Ukraine/Sweden exporting to the Netherlands/Germany.

In *Chapter 5*, it was determined that traditional coal-based steelmaking regions can switch to renewables-based production given adequate land, energy, and financial capital. Yet, it is regional trade partnerships, and strong carbon price signals that lay the foundations for green steel project investments for export-oriented industries. Besides, diversity in trade products (i.e., both green iron and green steel) and destination help to maintain supply chain resilience in the face of geopolitical risks. Relocation of iron and steel plants within national borders to tap into higher quality solar and wind resources is a viable means of maintaining market share with changing demand signals (i.e., for greener products). Whilst solar and wind energy offer scalable and rapidly deployable energy sources, an integrated energy system including mature zero-emissions sources of hydropower and nuclear power, is more robust in providing reliable, secure energy at a competitive price, especially in the short-term. Coal-based asset inertia may not be as significant as perceived; the strength of this opposing force depends on the age of the assets and the latest BF relines. These conclusions transcend the Ukrainian context (21.4 Mt steel produced, 15.7 Mt exported in 2021) to other iron ore-producing nations with export-oriented steel industries: for example, Turkey (40.4 Mt steel produced, 22.1 Mt exported), Brazil (36.2 Mt steel produced, 11.5 Mt exported), and Vietnam (23.0 Mt steel produced, 11.2 Mt exported) (worldsteel, 2022). In fact, the green steel transition model can be utilised by any locality/nation/region, regardless of the natural resource endowment and historical steel production.

The thesis also contains methodological contributions to steel decarbonisation literature, namely the facility-level green H₂-DRI-EAF optimisation model, and the green steel transition optimisation model, both publicly available through an open access licence. The applied use of machine learning to expand the spatial coverage of the facility-level analysis from 44 regions to over 300 deposits was also a novel means of carrying out a global analysis of renewables-based production costs. In general, the geospatial explicit supply chain approach highlighted the utility of systems engineering methods within

iron and steel sectorial analyses and provides a lens through which to evaluate various industrial decarbonisation challenges.

Several insights can be drawn from the results which have direct relevance for industry practitioners and policymakers. For steelmakers, the importance of regional partnerships to maintain market competitiveness in the clean energy transition emerged. Companies are urged to explore novel supply chain configurations, especially the utility of HBI trade in dislocating iron and steel production, based on dynamic local resource availability (renewable energy, iron ore, and scrap, among others) and market demands. For policymakers, this work reinforces the importance of financing instruments for low and near zero-emission technology investments in the form of incentive schemes (e.g., the United States' Inflation Reduction Act) or carbon taxes with appropriate border adjustments (e.g., the EU-ETS and CBAM). The strong inertia of steelmaking assets due to long lifetimes is an opposing force that must be overcome by favourable financing; prospective BF relining dates are critical milestones to alter the momentum of invested assets. Green iron/steel market coordination is called upon, that is, mechanisms for first mover supply-demand matching. Of note, the steel industry's transition would be supported by the removal of protectionist policies, and agreements on free trade under common emission accounting rules and low/near-zero emissions steel definitions. The public and private sectors both have a role to play in industrial coordination to establish the fundamental renewable energy system that will support the decarbonisation of energy-intensive industries. Following, finance should be targeted at removing potential supply chain blockages, e.g., electrolyser production, DRI furnace production, and DR-grade iron ore supply. This thesis is an academic output that has been informed by industry and framed by policy levers, and hence delivers pragmatic results.

6.3 Limitations and future work

Looking at the overall thesis, there are a few critical areas where the research was limited and future work is prompted. Firstly, the research only began to consider the complexity of geopolitical tensions (e.g. protectionist industrial policies, trade agreements that are perverse to decarbonisation objectives) related to steel production, which should be further explored at least qualitatively. In the present work, geopolitical factors were not considered in the global facility-based analysis (Chapter 3), by-design, to assess optimality on a pure techno-economic basis, whilst the research frameworks of both the binational supply chain analysis (Chapter 4) and green steel transition study (Chapter 5) were underpinned by regional trade considerations. To this end, a more holistic assessment framework for steel decarbonisation should be adopted to explore not just economically optimal supply chain configurations, but those that eliminate/minimise impacts on society (e.g., through labour and human rights maintenance, and local community engagement) and the environment (e.g., by preventing biodiversity loss, and air/noise/water pollution). The unintended consequences of resource shuffling could be politically, socially, and environmentally damaging. Questions have already emerged from other academics in response to the research, such as: *“Is there an optimal and equitable supply configuration? Can modern societies, confronted with significant geopolitical risks, accept such an optimal and equitable supply configuration?”* (Watari et al., 2023). Moreover, whilst industrial relocation

may be energetically and economically rational, trade-offs between holistic sustainability objectives, system resilience, and optimality must be assessed.

Secondly, the research identified a severe lack of spatially granular data on iron ore resources. Whilst climatic data to determine solar and wind potential is widely available at coordinate-level from multiple reputable sources, including ERA-5 and MERRA, data on iron ore quantity (including total reserve size and extraction rate) and quality (including ore type and Fe content) at mine-level could scarcely be sourced. There is certainly no globally available dataset; attaining iron ore mine data relies on investigating company reports which frequently do not even declare Fe content, nor ore type. This data limitation made iron ore cost estimation difficult as vast assumptions had to be made regarding the degree of beneficiation required. Information transparency by iron ore mining companies is crucial for more accurate assessments of steel decarbonisation potential, especially considering the enhanced iron ore quality required for direct reduction furnace production. Transparent global asset databases covering energy resources, power plants, and steel plants, have been incredibly useful inputs for industry decarbonisation modelling exercises, and the opportunity exists to expand the asset base to iron ore mines.

Finally, a global supply chain optimisation study is the next logical step in this body of work. In fact, the green steel transition model that underpinned the Ukrainian assessment was intentionally developed for global expansion. Accurate characterisation of dominant steel producers and consumers which had not yet been studied in detail, i.e., China, India, and the US, would be integral to assuring the model's validity. This spatial coverage expansion would enable important questions to be answered in the 1.5°C-aligned pathway to 2050. For example, is iron and steel production dislocation, and therefore green HBI trade corridors, essential for accelerating decarbonisation progress? To what extent do greenfield projects emerge, as well as intra-regional and/or inter-regional trade blocks? Consequently, global opportunities and risks for transitioning steel supply chains may be identified.

Appendix I: Supplementary Information to Chapter 3

A.i.1 Supplementary Results

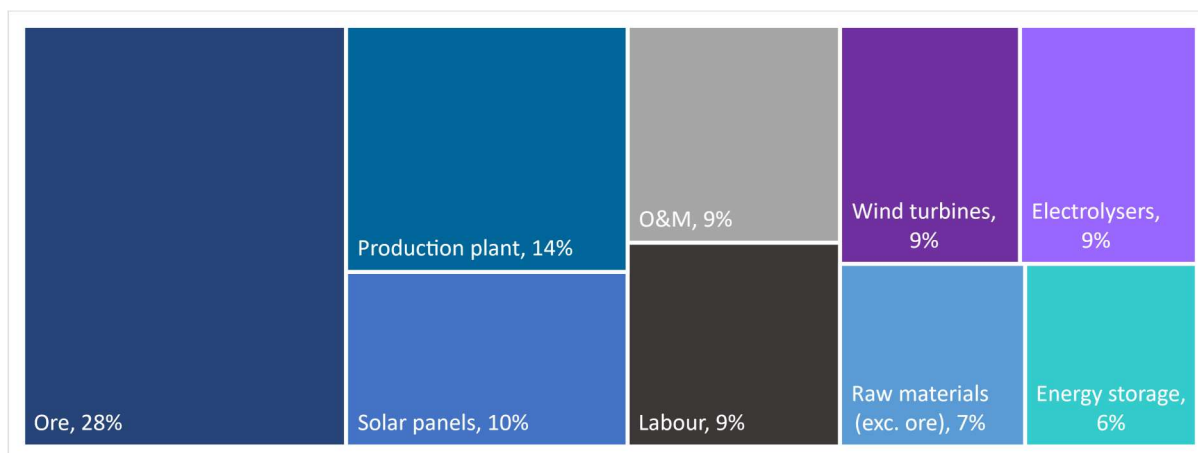


Figure S3.1 Green hydrogen-based steel cost structure in 2050, average across all locations (0% scrap)

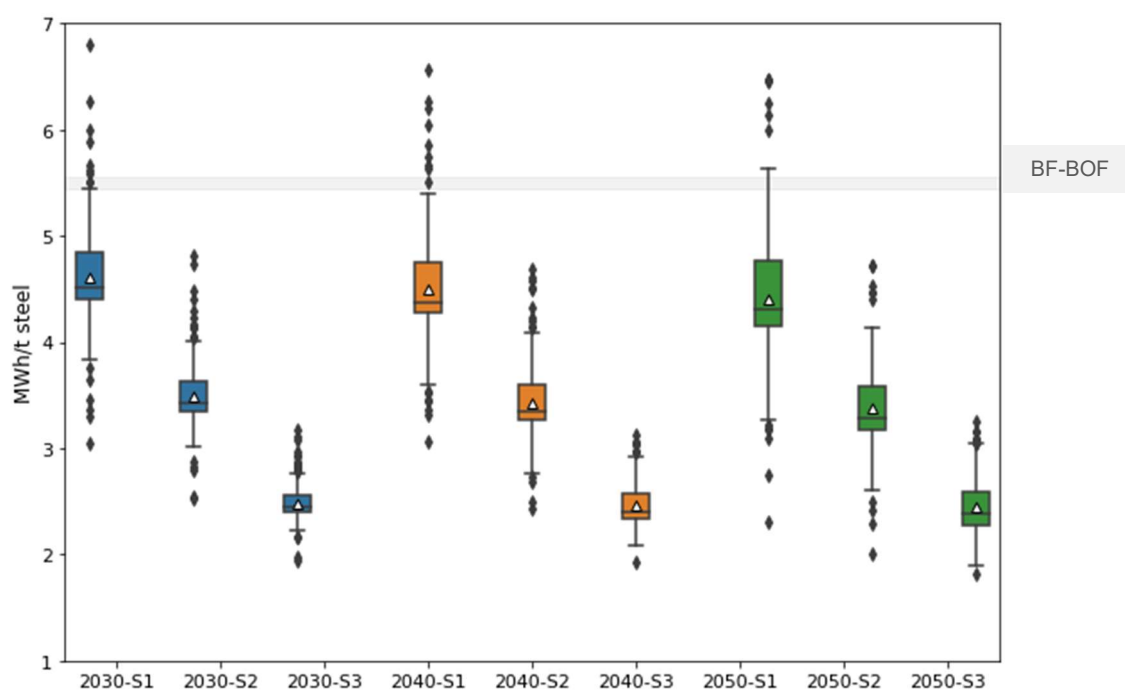


Figure S3.2 Energy-intensity of iron and steel production for all installation years and scrap charges (case S1 = 0% scrap, S2 = 25% scrap, S3 = 50% scrap)

Table S3.1 Renewable energy statistics for the 17 optimised countries

Country	Country code	mean hourly solar CF	median hourly solar CF	CoV hourly solar CF	mean monthly solar CF	median monthly solar CF	CoV monthly solar CF	mean hourly wind CF	median hourly wind CF	CoV hourly wind CF	mean monthly wind CF	median monthly wind CF	CoV monthly wind CF
Australia	AU	0.26	0.02	1.18	186.63	188.79	0.11	0.39	0.37	0.66	287.50	288.70	0.12
Brazil	BR	0.22	0.01	1.25	157.66	156.46	0.10	0.18	0.14	0.91	134.05	127.72	0.27
Canada	CA	0.15	0.00	1.54	111.48	116.72	0.31	0.33	0.27	0.86	239.83	235.26	0.16
Chile	CL	0.32	0.03	1.12	230.17	232.73	0.09	0.04	0.01	1.84	31.59	30.78	0.21
China	CN	0.22	0.01	1.29	163.46	164.52	0.13	0.33	0.28	0.77	241.61	245.79	0.20
Guinea	GN	0.19	0.00	1.30	141.97	136.94	0.12	0.11	0.07	1.08	77.28	69.48	0.29
India	IN	0.22	0.01	1.26	159.47	162.79	0.13	0.20	0.14	1.05	142.72	131.64	0.31
Iran	IR	0.30	0.03	1.13	217.12	220.20	0.08	0.24	0.18	0.85	176.83	176.41	0.20
Kazakhstan	KZ	0.20	0.02	1.27	147.29	158.47	0.25	0.41	0.39	0.53	296.82	297.66	0.12
Mexico	MX	0.23	0.01	1.25	171.19	172.45	0.11	0.13	0.09	1.34	97.14	95.08	0.20
Peru	PE	0.25	0.01	1.26	179.14	175.44	0.10	0.03	0.01	1.79	25.50	24.33	0.22
Russia	RU	0.14	0.01	1.50	100.89	98.85	0.42	0.28	0.25	0.72	207.46	205.20	0.17
Sweden	SE	0.13	0.00	1.68	91.34	85.82	0.52	0.26	0.22	0.78	193.31	186.61	0.20
Turkey	TR	0.25	0.03	1.22	184.58	185.10	0.18	0.19	0.10	1.18	135.10	139.16	0.24
Ukraine	UA	0.20	0.01	1.34	144.01	149.20	0.27	0.36	0.33	0.69	263.05	258.44	0.16
United States	US	0.21	0.01	1.33	154.42	158.91	0.18	0.32	0.28	0.75	236.07	236.22	0.16
South Africa	ZA	0.28	0.02	1.15	203.87	204.43	0.08	0.31	0.27	0.79	226.81	223.50	0.14

Table S3.2 Flexibility characteristics of the steel production system (projects installed in 2050, no scrap charging)

Country	Total H ₂ (t/t steel)	CGH ₂ (t/t steel)	% CGH ₂ of total H ₂	HDRI (t/t steel)	CDRI (t/t steel)	% CDRI of total DRI	Electrolyser oversizing factor	EAF oversizing factor
AU	0.06	0.03	45%	1.00	0.26	21%	2.04	1.17
BR	0.07	0.05	65%	0.95	0.31	24%	3.00	1.32
CA	0.07	0.03	38%	0.95	0.30	24%	2.03	1.26
CL	0.09	0.06	70%	1.01	0.25	20%	2.88	1.21
CN	0.07	0.03	48%	0.99	0.27	21%	2.38	1.20
GN	0.08	0.06	75%	0.97	0.29	23%	3.67	1.35
IN	0.08	0.05	69%	0.97	0.28	22%	3.14	1.27
IR	0.08	0.05	66%	0.95	0.30	24%	2.88	1.29
KZ	0.06	0.01	23%	1.01	0.24	19%	1.32	1.13
MX	0.08	0.05	67%	1.00	0.26	20%	3.20	1.23
PE	0.08	0.06	75%	0.97	0.28	22%	3.18	1.34
RU	0.06	0.02	37%	0.97	0.28	23%	1.77	1.21
SE	0.07	0.03	39%	0.97	0.28	22%	1.81	1.19
TR	0.08	0.05	60%	0.94	0.32	25%	2.77	1.26
UA	0.06	0.02	34%	1.02	0.23	19%	1.69	1.15
US	0.06	0.03	43%	0.99	0.26	21%	2.01	1.20
ZA	0.07	0.04	54%	0.98	0.27	22%	2.44	1.22

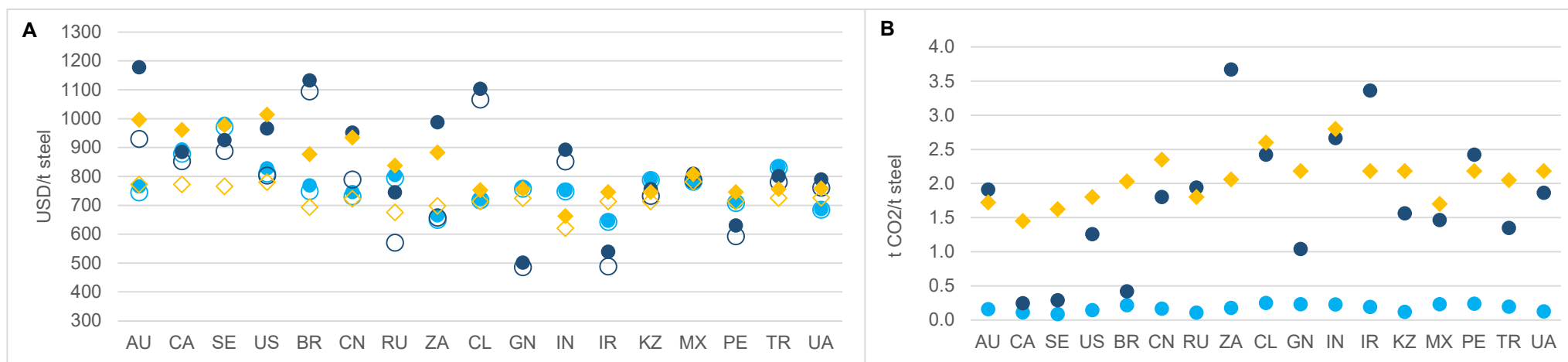


Figure S3.3 For 2030 project installation (no scrap): (a) Projected LCOS, with and without carbon taxes, and (b) CO₂ emissions intensity comparison across various steel production routes - (i) H₂-DRI-EAF with islanded energy system, (ii) H₂-DRI-EAF powered by national grid and (iii) conventional BF-BOF route.

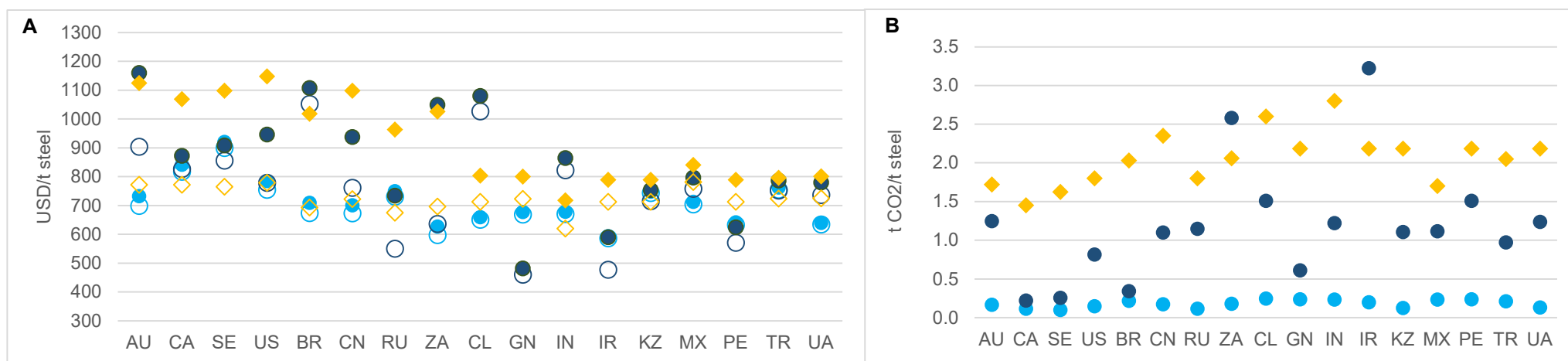
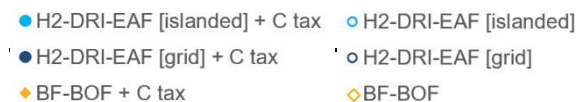


Figure S3.4 For 2040 project installation (no scrap): (a) Projected LCOS, with and without carbon taxes, and (b) CO₂ emissions intensity comparison across various steel production routes - (i) H₂-DRI-EAF with islanded energy system, (ii) H₂-DRI-EAF powered by national grid and (iii) conventional BF-BOF route.



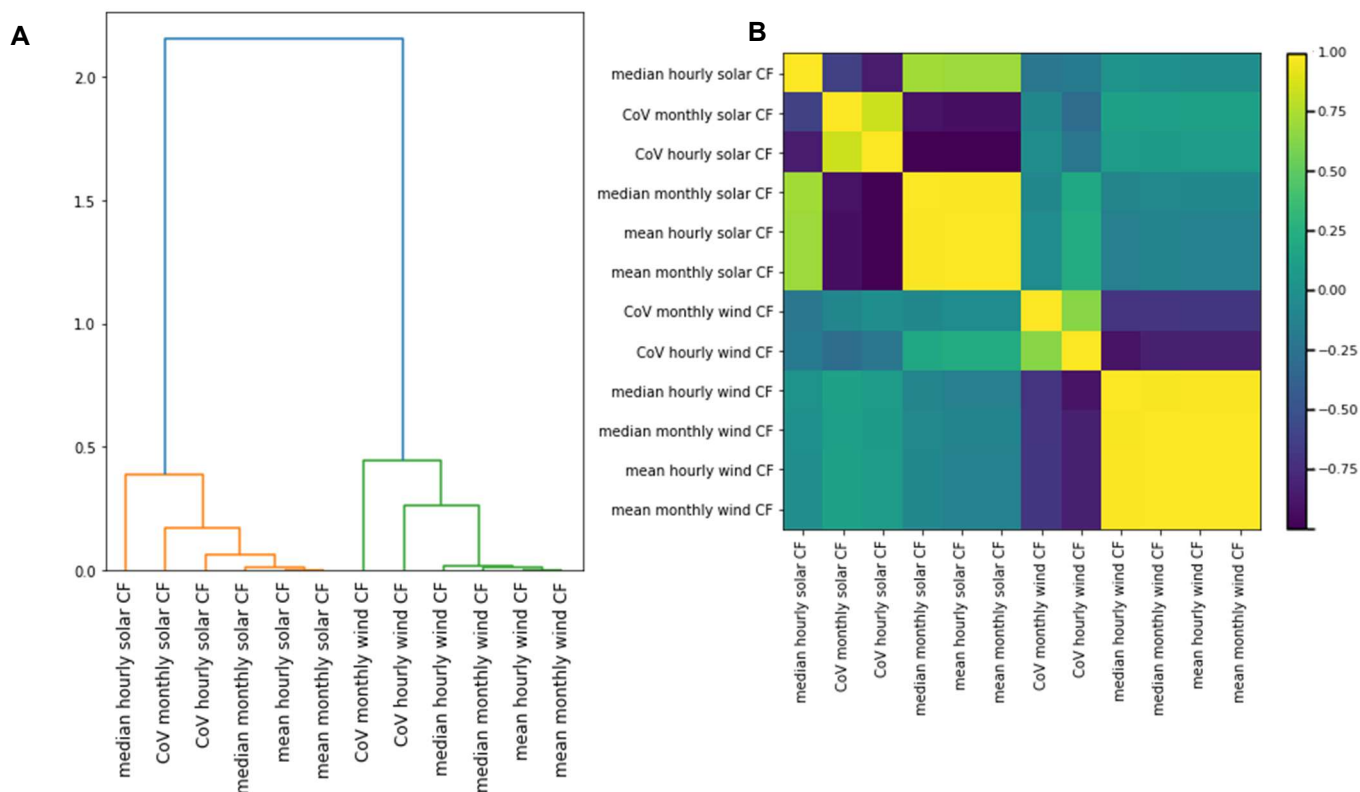


Figure S3.5 (a) Multicollinearity analysis, and (b) Correlation matrix, of renewable energy statistics.

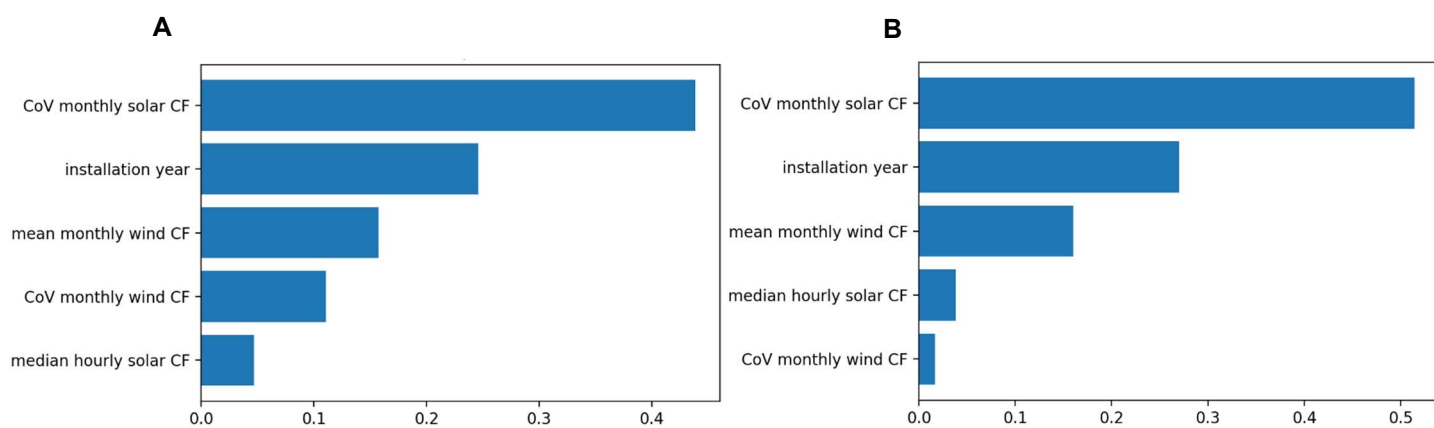


Figure S3.6 Feature importance for machine learning models for (a) LCOS (exc. ore) and (b) RE cost.

Table S3.3 Added ore and transport costs for LCOS at site, FOB and CFR economic assessments (2050, no scrap)

Country	LCOS, exc. ore	LCOS, inc. ore	LCOS FOB	LCOS CFR	Ore cost addition on top of LCOS at site	FOB cost increase from site costs (inc. ore)	CFR increase from FOB
AU	553	679	687	720	23%	1%	5%
BR	526	652	677	737	24%	4%	9%
CA	651	779	801	855	20%	3%	7%
CL	509	642	653	709	26%	2%	9%
CN	468	595	625	639	27%	5%	2%
GN	552	662	679	738	20%	3%	9%
IN	537	664	671	702	24%	1%	5%
IR	480	590	604	642	23%	3%	6%
KZ	471	702	745	805	49%	6%	8%
MX	550	675	686	729	23%	2%	6%
PE	531	639	651	706	20%	2%	8%
RU	650	757	820	874	16%	8%	7%
SE	473	598	614	659	27%	3%	7%
TR	682	802	809	875	18%	1%	8%
UA	579	705	719	767	22%	2%	7%
US	525	651	661	712	24%	2%	8%
ZA	599	725	779	825	21%	7%	6%

A.i.2 Supplementary Methods

Table S3.4 Production sub-systems with breakdown of processes and storage

Sub-system	Processes	Storage
RE supply + battery storage	- Solar energy delivery - Wind energy delivery - Li-ion battery charging and discharging	Li-ion battery storage
Hydrogen production and storage	- Water electrolysis - H₂ compression (200 bar) - Fuel cell power production	CGH ₂ storage
Ore mining and preparation	- Drilling and blasting - Loading and hauling - Crushing and screening - Beneficiation - Pelletising - Stacking and reclaiming	Ore pellet storage* Lump ore storage*
Ironmaking	- H₂ compression pre-DRI (2 bar) - H₂ heating pre-DRI (to 900°C) - Direct reduction of iron	Cold-DRI storage*
Steelmaking	- Cold-DRI heating (to 850°C) - Electric arc furnace - Continuous casting	Scrap storage* Lime, alloys storage* Steel storage*

*no energy or cost burdens associated with material storage

Table S3.5 Selected countries and key characteristics

Country	Alpha-2 code	No. regions	Economic status	Fe-content of extracted ore (U.S. Geological Survey, 2022)
Australia	AU	2	Advanced	0.62
Brazil	BR	3	Major emerging	0.63
Canada	CA	4	Advanced	0.60
Chile	CL	1	Emerging market/developing economy	0.63
China	CN	6	Major emerging	0.61
Guinea	GN	1	Emerging market/developing economy	0.66
India	IN	3	Emerging market/developing economy	0.63
Iran	IR	1	Emerging market/developing economy	0.66
Kazakhstan	KZ	1	Emerging market/developing economy	0.20
Mexico	MX	2	Emerging market/developing economy	0.65
Peru	PE	1	Emerging market/developing economy	0.69
Russia	RU	8	Major emerging	0.71
Sweden	SE	1	Advanced	0.70
Turkey	TR	1	Emerging market/developing economy	0.56
Ukraine	UA	1	Emerging market/developing economy	0.63
United States	US	4	Advanced	0.63
South Africa	ZA	4	Major emerging	0.64

Table S3.6 Key datasets for geospatial analysis

Data	Details	Sources
Solar and wind capacities	Hourly resource capacity based on 1kW capacity system and MERRA-2 climatic data. <i>Solar attributes: 1-axis rotation (azimuth), 10% system loss, 35° tilt, 180° azimuth.</i> <i>Wind attributes: 100m hub height, turbine model Vestas V90 2000.</i>	Renewables Ninja (Pfenninger & Staffell, 2016; Staffell & Pfenninger, 2016)
Iron ore deposit locations	Latitude and longitude of major global iron ore deposits.	Schulz and Briskey (2005), published by U.S. Geological Survey
Iron ore reserve characteristics	Extracted ore iron ore and reserve statistics, including overall quantity and iron ore content, presented at national level.	U.S. Geological Survey (2022) (and 5+ years of preceding annual publications)
Port locations	Latitude and longitude of global seaports, with classifications.	National Geospatial Intelligence Agency (2020)

Table S3.7 Mass loss rates in the ore preparation processes (Harvey, 2020)

Process	Mass losses
Crushing and screening	19%
Beneficiation	2.68% per ΔFe (%) in concentration
Pelletising	3%

Table S3.8 Ore mining and preparation process energy demand

Process	Energy demand	Unit	Reference
Drilling and blasting	1.28	kWh/t crushed ore	Norgate & Haque (2010)
Loading and hauling	25.58	kWh/t crushed ore	Norgate & Haque (2010)
Crushing and screening	6.42	kWh/t crushed ore	Norgate & Haque (2010)
Comminution (grinding + re-grinding)	27.36	kWh/t crushed ore	Palacios et al. (2019)
Concentration	0.85	kWh/t crushed ore- Δ Fe(%)	Palacios et al. (2019)
Pelletising	208.28	kWh/t pellet	Lv et al. (2019)
Stacking and reclaiming	1.28	kWh/t pellet or lump	Norgate & Haque (2010)

Table S3.9 Renewables technology cost and efficiency parameters

Parameter	Unit	2030	2040	2050	Reference
Solar PV panel cost	M\$/MW	0.594	0.461	0.327	(IRENA2019)
Wind turbine cost	M\$/MW	1.088	0.962	0.835	(IRENA2019)
Li-ion battery cost	M\$/MWh	0.207	0.182	0.156	Cole and Frazier (2020)
Electrolyser cost (low temp)	M\$/MW	0.385	0.340	0.295	(IEA2021c)
Fuel cell cost (low temp)	M\$/MW	0.457	0.267	0.218	Whiston et al. (2019)
Electrolyser efficiency (low temp, alkaline)	%	0.680	0.715	0.750	IEA (2019)
FC efficiency (low temp)	%	0.600	0.620	0.640	IEA (2015)

Battery, electrolyser, and fuel cells were assumed to have to be replaced twice in project lifetime, whereas all other technology pertained lifetimes that equalled or exceeded 20 years.

Table S3.10 Resource consumption parameters

ENERGY CONSUMPTION	Rate	Unit	Reference
CGH ₂ compression (200 bar)	2.87	MWh/t CGH ₂	Devlin and Yang (2022)
Direct reduction of iron (H ₂ feedstock)	48.13	kg H ₂ /t DRI	Devlin and Yang (2022)
H ₂ heating pre-DRI	1606.10	MJ/t DRI	Devlin and Yang (2022)
H ₂ compression pre-DRI	0.06	MWh/t DRI	Devlin and Yang (2022)
HBI briquette compression	0.01	MWh/t HBI	own calculations, based on data from (Lohmeier et al., 2020)
HBI/CDRI heating	152.78	MWh/t HBI/CDRI	own calculations, based on data from (Midrex, 2018)
Continuous casting	0.01	MWh/t steel	Devlin and Yang (2022)
EAF steelmaking			Kirschen et al. (2021)
- 0% scrap	0.75	MWh/t steel	
- 25% scrap	0.73	MWh/t steel	
- 50% scrap	0.71	MWh/t steel	
MATERIAL CONSUMPTION			
Ore demand			own calculations
- 0% scrap	1.73	dmt t/t steel	
- 25% scrap	1.24	dmt t/t steel	
- 50% scrap	0.79	dmt t/t steel	
Scrap demand			own calculations
- 0% scrap	0.00	t/t steel	
- 25% scrap	0.30	t/t steel	
- 50% scrap	0.57	t/t steel	
Lime demand			Kirschen et al. (2021)
- 0% scrap	50.00	kg/t LS	
- 25% scrap	49.50	kg/t LS	
- 50% scrap	49.00	kg/t LS	
Alloys	11.00	kg/t LS	Vogl et al. (2018)
Electrodes	2.00	kg/t LS	Vogl et al. (2018)
DRI metallisation rate (metallic Fe/total Fe)	94%		Kirschen et al. (2021)
EAF metal yield (mass of charged metal/mass of tapped steel)			
- 0% scrap	85%		own calculations
- 25% scrap	87%		own calculations
- 50% scrap	89%		own calculations
LAND CONSUMPTION			
Solar PV panels	0.02	km ² /MW	NREL (2022)
Wind turbines	0.12	km ² /MW	NREL (2022)
EMISSION-INTENSITY			
Solar PV panels	48	g CO ₂ -e/kWh	Pehl et al. (2017)
Wind turbines	12	g CO ₂ -e/kWh	Pehl et al. (2017)

Table S3.11 Economic parameters

Item	Value	Unit	References and notes
Real discount rate	8.00%	/yr	
Project lifetime	20	years	

OPEX

Scrap	265	\$/t	Facchini et al. (2021); Vogl et al. (2018)
Lime	121	\$/t	Vogl et al. (2018)
Alloys	2,397	\$/t	Vogl et al. (2018)
Carbon (graphite electrodes)	5,395	\$/t	Vogl et al. (2018)
Labour - ironmaking (inc. H ₂ production)	19	\$/t DRI	OECD (2021a); Vogl et al. (2018); Wood et al. (2020)
Labour - steelmaking (EAF, casting)	53	\$/t steel	OECD (2021); Vogl et al. (2018); Wood et al. (2020)
Maintenance	2%	of CAPEX	Wood et al. (2020)

Infrastructure CAPEX

DRI shaft furnace	310	\$/Mt rated DRI capacity	Vogl et al. (2018)
EAF unit - continuous mode	283	\$/Mt rated steel capacity	Facchini et al. (2021); Steelonthenet.com (2022); Vogl et al. (2018)
Casting	0.945	\$/t LS per hour (peak capacity)	Xylia et al. (2018)
CGH ₂ plant (200 bar)	2.064	\$/t H ₂ per hour (peak capacity)	Abdin et al. (2021)
CGH ₂ storage vessel (200 bar)	0.70	\$/t CGH ₂ stored (peak capacity)	Abdin et al. (2021)
H ₂ compressor (2 bar)	8.4074x + 4.5351	\$/Mt rated DRI capacity where $x = \text{DRI production (Mtpa)}$	Luyben (2018)

Table S3.12 Dry bulk freight rates

(a) Constant rates

Transportation cost item	Value	Unit	Reference
Rail freight	0.024	USD/t-km	van der Meulen et al. (2020) Bureau of Infrastructure Transport and Regional Economics (BITRE) (2017)
Panamax charter rate (exc. fuel)	0.0008	USD/t-km	BIMCO (2021)
Panamax NH ₃ consumption rate	0.22	t/nm	MAN Diesel and Turbo (2014)
Port handling fee (load/unload)	7.00	USD/t	van der Meulen et al. (2020) Abu Dhabi Ports (2021)

(b) Time-variable rates

	2030	2040	2050		
NH ₃ costs	713	570	460	\$/t NH ₃	IRENA (2022b)
Fuel consumption (SOFC)	364	354	344	g/kWh	Devlin and Yang (2022)

Table S3.13 Industrial electricity tariffs

Country ID	Country	Industrial electricity tariffs, 2018 (IEA, 2020d)	Data gaps filled by adjusted Cable.co.uk data*
AU	Australia	n/a	108.29
BR	Brazil	168.67	
CA	Canada	83.95	
CL	Chile	158.65	
CN	China	89.36	
GN	Guinea	n/a	20.62
IN	India	110.12	
IR	Iran	n/a	27.98
KZ	Kazakhstan	49.64	
MX	Mexico	89.53	
PE	Peru	n/a	50.34
RU	Russia	41.23	
SE	Sweden	87.2	
TR	Turkey	83.95	
UA	Ukraine	90.44	
US	United States	69.34	
ZA	South Africa	64.16	

*for the 4 countries where IEA data was not available, data for global household energy prices from Cable.co.uk (2021) was adjusted using OECD average difference between household and industrial electricity tariffs (-37%) (IEA, 2020a)

Table S3.14 BF-BOF emissions intensity (Hasanbeigi & Springer, 2019)

Country	t CO2/t steel
AU	1.72
BR	2.03
CA	1.45
CL	2.60
CN	2.35
GN	2.18
IN	2.80
IR	2.18
KZ	2.18
MX	1.70
PE	2.18
RU	1.80
SE	1.63
TR	2.05
UA	2.18
US	1.80
ZA	2.06

Italicised = economy-wide approximation

Table S3.15 BF-BOF production costs (Transition Zero, 2022)

Country	BF-BOF site costs (USD/t steel)	Assumptions
AU	773	'advanced' economy average
BR	694	
CA	773	'advanced' economy average
CL	714	'developing' economy average
CN	723	
GN	724	no steel production - assume global average
IN	621	
IR	714	'developing' economy average
KZ	714	'developing' economy average
MX	782	
PE	714	'developing' economy average
RU	676	
SE	766	EU data from Medarac et al. (2020) (exc. credits) plus global avg. 2020-21 delta from Transition Zero (2022)
TR	725	
UA	726	
US	780	
ZA	698	'major emerging' economy average

Table S3.16 Carbon prices (IEA, 2021e)

C price (\$/t CO₂) based on economy – net zero scenario			
<i>Economy classification</i>	<i>2030</i>	<i>2040</i>	<i>2050</i>
Advanced	130	205	250
Major emerging	90	160	200
Emerging market/developing economy	15	35	55

Table S3. 17 Regionally variable scrap prices based on trade volumes and economic value of flows under HS 720429 - Waste or scrap, of alloy steel, other than stainless (UNComtrade, 2021)

Country	Import Qty (t)	Export Qty (t)	Trade position	Import price (USD/t, 2021 dollars)	Export price (USD/t, 2021 dollars)	Domestic price** (USD/t, 2020 dollars)
Australia	106,442	138,220	Exporter	491	444	424
Brazil	6,860	88,481	Exporter	1355	397	380
Canada	153,052	995,875	Exporter	256	494	472
Chile	6,763	21,699	Exporter	326	405	387
China	96,807	141	Importer	754	222	212
Guinea*	-	-	Importer	-	-	417
India	98,079	1,403	Importer	758	468	447
Iran*	-	-	Importer	-	-	417
Kazakhstan*	-	-	Importer	-	-	417
Mexico	94,772	234,685	Exporter	375	413	395
Peru	109,831	19,028	Importer	497	453	433
Russia	410,136	9,300	Importer	358	654	624
South Africa*	15,105	-	Exporter	163	-	417
Sweden	14,772	68,709	Exporter	1126	372	355
Turkey	125,741	11,102	Importer	427	1093	408
Ukraine	459	91	Importer	759	559	534
United States	696,763	903,352	Exporter	464	455	434

*assumed average medium quality scrap price due data unavailability

**assumed export market drives the domestic price, excluding Turkey, the largest global scrap steel importer

Table S3.18 Regionally variable steelworker wages

	Average wage (before tax)	Steelworker wage (before tax)		Personal Income Tax Rate (highest)	Steelworker hourly rate, inc. tax
Source	(World Bank Group, 2022b)	30% increase above average (Wood et al., 2020)		(PwC, 2023)	Calculation
Unit	\$/year	\$/year	\$/hr	% of income	\$/hr
AU	53620	69706	36.31	45%	52.64
BR	7820	10166	5.29	28%	6.75
CA	43540	56602	29.48	33%	39.21
CL	12990	16887	8.80	40%	12.31
CN	10520	13676	7.12	45%	10.33
GN	960	1248	0.65	40%	0.91
IN	1890	2457	1.28	43%	1.83
IR	3290	4277	2.23	35%	3.01
KZ	8710	11323	5.90	10%	6.49
MX	8750	11375	5.92	35%	8.00
NZ	41480	53924	28.09	39%	39.04
PE	6000	7800	4.06	30%	5.28
RU	10740	13962	7.27	13%	8.22
ZA	6090	7917	4.12	45%	5.98
SE	54740	71162	37.06	52%	56.34
TR	9070	11791	6.14	40%	8.60
UA	3570	4641	2.42	18%	2.85
US	64650	84045	43.77	37%	59.97

Table S3.19 Labour intensities

Process	Labour intensity	Source
Green H ₂ production	2 hours/kW installed electrolyzers	Own calculations using data from Leguijt et al. (2021), considering labour demand for RE generation and electrolysis parts of value chain.
DR ironmaking	0.22 hours/t DRI	Own calculations using data from Wood et al. (2020).
EAF steelmaking	0.49 hours/t steel	

Appendix II: Supplementary Information to Chapter 4

A.ii.1 Supplementary Methods

Energy Pathways

Table S4.1 below explicates the energy pathway, from VRE to end-use, when performed in Australia (differentiated by VRE_{on} or VRE_{off}) or Japan. Flexible processes were only supplied by direct VRE during VRE_{on} in Australia, whilst inflexible processes had an additional supply route during VRE_{off}. The energy pathway is shown for both Australia- and Japan-based production, where applicable.

Table S4.1 Energy pathways, dependent on process flexibility and country

Process	Energy type	Flexibility	Country	Supply route - Aus (VRE _{on})	Supply route - Aus (VRE _{off}) or Japan
Water electrolysis	Electricity (DC)	Flexible	AU	Direct VRE	-
H ₂ liquefaction	Electricity (AC)	Flexible	AU	Direct VRE	-
CGH ₂ storage compression	Electricity (AC)	Flexible	AU	Direct VRE	-
NH ₃ synthesis	Electricity (AC)	Inflexible	AU	Direct VRE	CGH ₂ -FC
NH ₃ cracking	Thermal	Inflexible	JP	-	VRE-Electrolysis-NH ₃
DRI	H ₂ feedstock	Inflexible	AU	Direct VRE	VRE-Electrolysis-CGH ₂ -FC
	H ₂ feedstock	Inflexible	JP	-	VRE-Electrolysis-LH ₂ /NH ₃ -regasification/cracking
H ₂ compression pre-DRI	Electricity (AC)	Flexible	AU	Direct VRE	-
	Electricity (AC)	Inflexible	JP	-	VRE-Electrolysis-LH ₂ /NH ₃ -FC
H ₂ heating pre-DRI	Electricity (AC)	Inflexible	AU	Direct VRE	-
	Thermal	Inflexible	AU	-	VRE-Electrolysis-CGH ₂ -combustion
	Thermal	Inflexible	JP	-	VRE-Electrolysis-LH ₂ /NH ₃ -combustion
EAF	Electricity (AC)	Inflexible	AU	Direct VRE	VRE-Electrolysis-CGH ₂ -FC
	Electricity (AC)	Inflexible	JP	-	VRE-Electrolysis-LH ₂ /NH ₃ -FC
Casting	Electricity (AC)	Inflexible	AU	Direct VRE	VRE-Electrolysis-CGH ₂ -FC
	Electricity (AC)	Inflexible	JP	-	VRE-Electrolysis-LH ₂ /NH ₃ -FC
Marine transportation	Electricity (AC)	Inflexible	AU	Direct VRE	VRE-Electrolysis-CGH ₂ -FC
	Electricity (AC)	Inflexible	JP	-	VRE-Electrolysis-LH ₂ /NH ₃ -FC

Homer Pro energy calculations

Total daily electricity demand was inputted as deferrable load in Homer Pro, the sum of all system demands (excluding external iron ore mining and water desalination processes). All loads were converted to DC due to the pairing of solar electricity DC outputs and the central electrolyser DC load. System flexibility of 5% unmet electric load was given to rationalise for the constant daily load profile throughout the year, hence the lack of seasonal production consideration. If we had adopted a seasonally variant diurnal demand profile by minor adjustment of the assumed steel output, this 5%

unmet electric demand would likely not be needed to achieve similar LCOE to what is currently projected.

The deferrable peak load, required by Homer Pro, was determined by:

$$\text{Peak load (kW)} = \text{daily load (kWh/d)} / \text{VRE}_{on} \text{ (hrs/day)} \quad (\text{Eqn S4.1})$$

The storage capacity (a system flexibility constraint, required by Homer Pro) differed according to the case. For SC1-LH₂, as all loads were flexible, no restrictions existed for when load could be served, therefore

$$\text{Storage capacity}_{\text{SC1-LH}_2} \text{ (kWh)} = \text{daily load (kWh)} \quad (\text{Eqn S4.2})$$

Otherwise, inflexible processes restricted supply and the storage capacity was determined by the flexible CGH₂ and LH₂ storage:

$$\begin{aligned} \text{Storage capacity}_{\text{SC2-LH}_2, \text{SC3-LH}_2} \text{ (kWh)} = \text{energy needed to} \\ \text{(a) produce the H}_2 \text{ to be stored by CGH}_2 \text{ and LH}_2, \text{ and} \\ \text{(b) run the compression for operating CGH}_2 \text{ and liquefier} \\ \text{for operating LH}_2 \end{aligned} \quad (\text{Eqn S4.3})$$

$$\begin{aligned} \text{Storage capacity}_{\text{NH}_3} \text{ (kWh)} = \text{energy needed to} \\ \text{(a) produce the H}_2 \text{ to be stored by CGH}_2 \text{ and} \\ \text{(b) run the compression for operating CGH}_2 \end{aligned} \quad (\text{Eqn S4.4})$$

Aspen Plus calculations

(a) The DRI process

The DRI process outlined in Figure S4.1, following the design of Krüger et al. (2020), was simulated in Aspen Plus using the SOLIDS property method. The reduction furnace was modelled by a adiabatic RStoic reactor (primarily for heat balance calculations), using surplus H₂ as heat carrier (with heat supplied through the pre-DRI H₂ heater, following an exchanger for heat recovery) to sustain the reduction reactions. Pressure drop in the furnace was considered, through a pre-DRI compression step to raise the pressure from 1 bar to 2 bar, although the operating pressure of the furnace was taken as 1 bar as a simplifying approximation. To estimate the temperature of the gaseous product of the furnace for an intended solid product temperature (850°C) that is expected to materialise in a adequately designed furnace, a heater (cooler) was applied to the solid (gaseous) product (not shown in Figure S4.1). The heater was specified with the intended solid product temperature (see Table S4.2) while the cooler's duty was set to be identical to that of the heater (through imposing a design specification in Aspen Plus). This way, the heat balance of the furnace was maintained.

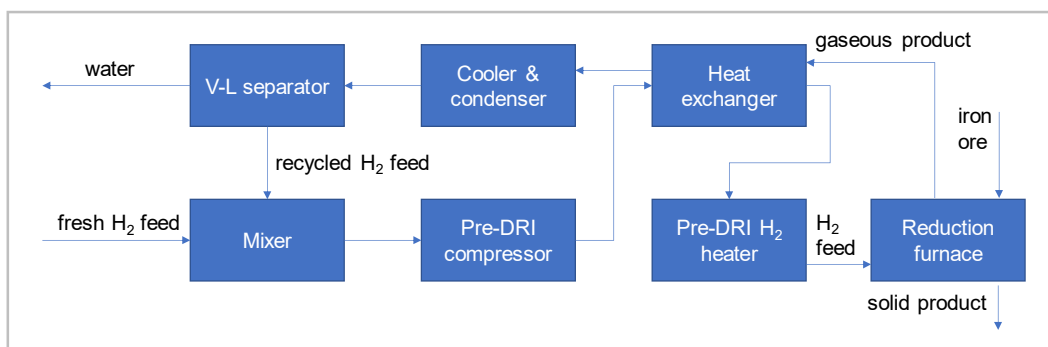


Figure S4.1 Block diagram of the DRI process simulated in Aspen Plus

Key simulation settings and results are given in Table S4.2. Note that the above-described process has a high-temperature output of reduced iron, ideal for directly feeding into the down-stream EAF process. In supply chain SC2, the thermal energy contained in the hot DRI product flow would not enter the EAF as the two processes were at different locations; the implications of this difference, as well as the requirements of the briquetting process, were ignored in this study. Furthermore, mass losses of iron were not considered in the conversion from sponge iron (Fe/FeO) to liquid steel (LS), then SFS.

Table S4.2 Aspen Plus simulation details for the DRI process

Simulation settings	
Iron ore feed rate and temperature	1500 kg/hr, 20 °C
Composition of iron ore (weight%)	95% of Fe ₂ O ₃ , 5% of inert (represented by SiO ₂)
Furnace operating pressure	1 bar
Metallisation (FeO to Fe conversion) rate	94%
Fresh H ₂ feed rate, temperature and pressure	51.4 kg/hr, 80°C, 1 bar
H ₂ conversion rate in furnace	30.5%
Solid product temperature	850°C
"H ₂ +steam" stream condensing temperature	40°C
Results	
H ₂ heating requirement	0.4446 MW
H ₂ compression work requirement	0.0642 MW
Temperature of gaseous outlet flow of the furnace	338°C
Solid products	Fe = 936.9 kg/hr; FeO = 76.9 kg/hr; SiO ₂ = 75 kg/hr

(b) NH₃ cracking

The NH₃ cracking reactor was modelled in Aspen Plus with the RStoic reactor model and the SKR physical property model. The reactor was assumed to operate isothermally. Before entering the reactor, liquid NH₃ was assumed to be pumped and pre-heated to the reactor conditions (see Table S4.3). Following pumping and prior to preheating, the NH₃ feed was assumed to reach 20 °C in gaseous state by absorbing heat from the ambient environment, free of energy cost. Heat recovery from cooling the reactor effluent and from the combustion of unconverted NH₃ and unrecovered H₂ was considered to counterbalance the heat required for pre-heating the feed and for maintaining the temperature of the

endothermic cracking reaction. The pumping energy requirement was negligible compared to the heating demand and was therefore not included in the assessment.

Key simulation and calculation settings, similar to those adopted by Giddey et al. (2017), are given in Table S4.3.

Table S4.3 Simulation and calculation details for NH₃ cracking

Simulation/calculation settings	
Reactor temperature	400 °C
Reactor pressure	8 bar
NH ₃ cracking conversion	95%
H ₂ product recovery	85%
Heating efficiency	85%
Target temperature of reactor effluent cooling for heat recovery	80 °C
Effective heat recovery ratio (from combustion of residual NH ₃ and H ₂ and from reactor effluent)	85%
Results – per tonne NH ₃ feed	
Total heating requirement	4556.47 MJ
Sensible heat recovered from reactor effluent	925.97 MJ
Heat recovered from the combustion of residual NH ₃ and H ₂	3370.44 MJ
Net heating requirement	260.05 MJ (0.072 MWh)

(c) CGH₂ compression work

Compression of H₂ was modelled via a 5-stage compressor with equal pressure ratio, inter-stage cooling temperature = 50°C, isentropic efficiency = 85%, mechanical efficiency = 95%, physical property model = SRK.

Shipping fuel consumption calculations

Specific fuel consumption (SFC) was particular to the vessel propulsion system, calculated according to Equation S4.5. We have taken an average 85% propulsion load factor; a measure of the load the fuel cell is operating at, in relation to the specified maximum continuous rating (SMCR). Note that PEMFC runs most efficiently at 10-25% load factor whilst SOFC runs most efficiently at 25-35% load factor.

$$SFC (g/kWh) = \frac{\text{correction factor}}{LHV_{fuel} \left(\frac{kW}{kg} \right) \div 1000 \frac{g}{kg} \times \eta} \quad (\text{Eqn S4.5})$$

where:

correction factor = 1.19 for PEMFC and 1.09 for SOFC (Kim et al., 2020) based on 85% propulsion load

LHV = 33.33kWh/kg for H₂, 5.17kWh/kg for NH₃

η = propulsion system efficiency (fuel cell (68% in 2030, 72% in 2050), inverter (95%), and electric motor (98%))

The fuel consumption due to propulsion load was specific to the vessel propulsion system and route, calculated by:

$$F_{\text{journey}} (t/\text{journey}) = \quad (\text{Eqn S4.6})$$

$$[SFC \left(\frac{g}{kWh} \right) \times \text{power} (kW) \times \frac{\text{distance} (nm/\text{journey})}{\text{speed} \left(\frac{nm}{h} \right)} \times 10^{-6} \left(\frac{t}{g} \right) \div (1 - BOG (\%))] \times 2$$

where:

power = propulsion power at 85% SMCR, i.e., 15% specified engine margin

distance = nautical distance from Port Hedland to Osaka + 15% sea margin

speed = speed of vessel

BOG = portion of initial mass lost over journey due to boil off gas, calculated using 0.2%/day for LH₂ (Wijayanta et al., 2019) and 0.02%/day for NH₃ (Al-Breiki & Bicer, 2020b). BOG losses were conservative for fuel as the decreasing daily mass due to consumption of fuel is not considered.

Shipping vessel specifications are detailed in Table S4.4. Note that propulsion power was later equalised on an 85% SMCR basis:

$$\text{Power}_{85\%SMCR} = \text{Power}_{X\%SMCR} \times \frac{85}{X} \quad (\text{Eqn S4.7})$$

Table S4.4 Shipping vessel specifications

Export	Vessel	dwt	Power (kW)	Specified engine margin	Speed (nm/h)	Reference
Iron ore	Dry bulk carrier Newcastlemax	205000	17180	10%	14.7	(MAN Diesel and Turbo, 2014)
HBI, steel	Dry bulk carrier, Panamax	75000	9470	10%	14.5	(MAN Diesel and Turbo, 2014)
LH ₂ , LNH ₃	Liquefied gas tanker, 160,000m ³	31000	27000	0%	18	(Yoshino et al., 2012) (Al-Breiki & Bicer, 2020b)

The propulsion load factor is distinct from the cargo carrying capacity. The former refers to the engine output whilst the latter refers to the amount of usable vessel space for exported goods. We have assumed a cargo carrying capacity of 90%. Both the laden (with cargo) and ballast (without cargo) journeys are considered. In the ballast journey, water effectively replaces the weight of cargo and equal propulsion power is required. The number of journeys is specific to the vessel, export and year, calculated by:

$$\text{journeys}_{\text{dry bulk}} (\text{no./year}) = (\text{total annual exports}) (t) \div \text{payload}_{\text{dry bulk}} (t/\text{vessel}) \quad (\text{Eqn S4.8})$$

$$\begin{aligned} \text{journeys}_{\text{gas tanker}} (\text{no./year}) = \\ (\text{total annual exports} + \text{BOG losses}) (t) \div \text{payload}_{\text{gas tanker}} (t/\text{vessel}) \end{aligned} \quad (\text{Eqn S4.9})$$

where:

$$\text{payload}_{\text{gas tanker}} (t) = 160,000\text{m}^3 \times \rho_{\text{fuel}} (\text{kg/m}^3) \times 90\%$$

$$\text{payload}_{\text{dry bulk}} (t) = ((\text{dwt} \times 90\%) - F_{\text{journey}}) \times 90\%$$

The journey duration is a function of the vessel speed:

$$\text{duration} (\text{days}) = \text{distance} (nm/\text{journey}) \div \text{speed}_{\text{vessel}} (nm/h) \div 24 (h/\text{day}) \quad (\text{Eqn S4.10})$$

The number of journeys and each journey's duration can then be used to determine the number of vessels in a fleet:

$$\text{vessels in fleet (no.)} = (\text{journeys (no.)} \times (\text{duration (days)} + 2) \times 2) \div 365.25 \quad (\text{Eqn S4.11})$$

Combined energy data and formulae

Table S4.5 specifies the energy demand formulae for end-uses powered by direct VRE or an energy vector (H_2 or NH_3); the latter has been separated into key categories: H_2 for feedstock, H_2 or NH_3 for power, H_2 or NH_3 for heat, and H_2 or NH_3 for mobility.

Energy consumption from H_2/NH_3 demand was determined by:

$$E (\text{MWh}) = \text{H}_2 \text{ demand (t)} \times \text{electrolysis energy demand (MWh/t H}_2\text{)} \quad (\text{Eqn S4.12})$$

$$E (\text{MWh}) = \text{H}_2 \text{ demand (t)} \times \text{H}_2/\text{NH}_3 (\text{t/t}) \times \text{electrolysis energy demand (MWh/t H}_2\text{)} \quad (\text{Eqn S4.13})$$

where:

H_2/NH_3 = mass conversion rate

$$= 0.002 (\text{g H}_2/\text{mol}) \times 1/0.017 (\text{g NH}_3/\text{mol}) \times 3/2 (\text{moles H}_2/\text{moles NH}_3)$$

$$= 0.176 (\text{i.e., H}_2 \text{ constitutes 17.6\% of ammonia by mass})$$

Note that VRE_{on} and VRE_{off} are only specified for inflexible processes in Australia which require constant load, 2030 and 2050 are only specified for processes which change in energy demand over time, and steel refers to semi-finished product (bloom, billet, or slab).

Table S4.5 Energy modelling formulae

Direct VRE (AU): $E_{\text{annual}} (\text{MWh}) = \text{demand rate (MWh/t)} \times \text{quantity (t H}_2/\text{NH}_3/\text{SFS})$						
Applicable processes	Energy vector	SC	Unit	Demand (MWh/unit)	Source	Qty (annual basis)
H_2 liquefaction	LH_2	SC1,2,3	t H_2	10 (2030) 6 (2050)	Berstad et al. (2019)	H_2 for export and shipping fuel
NH_3 synthesis (VRE_{on})	NH_3	SC1,2,3	t NH_3	0.7	Nayak-Luke et al. (2018)	NH_3 for export and shipping fuel x (VRE_{on} (hrs)/24)
CGH ₂ storage compression	LH_2	SC2	t H_2	2.68	Aspen Plus Model	H_2 heating pre-DRI (VRE_{off}) + [H_2 for DRI x (VRE_{off} (hrs)/24)]
		SC3				H_2 heating pre-DRI (VRE_{off}) + EAF (VRE_{off}) + casting (VRE_{off}) + [H_2 for DRI x (VRE_{off} (hrs)/24)]
	NH_3	SC1				H_2 for NH_3 synthesis power (VRE_{off}) + H_2 as synthesis feed (VRE_{off})
		SC2				H_2 for NH_3 synthesis power (VRE_{off}) + H_2 to be synthesised (VRE_{off}) + H_2 heating pre-DRI (VRE_{off}) + [H_2 for DRI x (VRE_{off} (hrs)/24)]
		SC3				H_2 for NH_3 synthesis power (VRE_{off}) + H_2 to be synthesised (VRE_{off}) + H_2

						heating pre-DRI (VRE _{off}) + EAF (VRE _{off}) + casting (VRE _{off}) + [H ₂ for DRI x (VRE _{off} (hrs)/24)]
H ₂ compression pre-DRI	LH ₂ , NH ₃	SC2,3	t steel	0.06	Aspen Plus Model	steel produced x (VRE _{on} (hrs)/24))
H ₂ heating pre-DRI (VRE _{on})	LH ₂ , NH ₃	SC2,3	t steel	0.45	Aspen Plus Model	steel produced x (VRE _{on} (hrs)/24))
EAF (VRE _{on})	LH ₂ , NH ₃	SC3	t steel	0.75	Kruger et al. (2020)	steel produced x (VRE _{on} (hrs)/24))
Casting (VRE _{on})	LH ₂ , NH ₃	SC3	t steel	0.01	IEA Environmental Projects (2013)	steel produced x (VRE _{on} (hrs)/24))
H₂ for feedstock (AU/JP): $H_{2,annual} (t\ H_2) = demand\ rate\ (kg\ H_2/t) \times quantity\ (t) \times 10^{-3}$						
Applicable processes	Energy vector	SC	Unit	Demand (kg H ₂)	Source	Qty (annual basis)
DRI	LH ₂ , NH ₃	SC1,2,3	t steel	51.98	Aspen Plus Model	steel produced
H₂ or NH₃ for heat (AU/JP): $H_{2,annual} (t\ H_2\ or\ NH_3) = demand\ rate\ (kg\ H_2\ or\ NH_3/t) \times quantity\ (t) \times 10^{-3}$						
Applicable processes	Energy vector	SC	Unit	Demand (kg H ₂ or NH ₃ /unit)	Source	Qty (annual basis)
NH ₃ cracking	NH ₃	SC1	t steel	5.98 kg NH ₃	Aspen Plus Model	steel produced
H ₂ heating pre-DRI (JP)	LH ₂	SC1	t steel	15.75 kg H ₂	LHV-based combustion calculation with 85% efficiency	steel produced
	NH ₃	SC1		101.59 kg NH ₃		steel produced
H ₂ heating pre-DRI (VRE _{off})	LH ₂ , NH ₃	SC2,3		15.75 kg H ₂		steel produced x (VRE _{off} (hrs)/24))
H₂ for power (AU): $H_{2,annual} (t\ H_2) = demand\ rate\ (kg\ H_2/t) \times quantity\ (t) \times 10^{-3}$						
Applicable processes	Energy vector	SC	Unit	Demand (kg H ₂ /unit)	Source	Qty (annual basis)
NH ₃ synthesis (VRE _{off})	NH ₃	SC1	t NH ₃	34.94 (2030) 32.76 (2050)	Nayak-Luke et al. (2018) for power required + FC efficiency	H ₂ for export and shipping fuel x (VRE _{off} (hrs)/24)
EAF (VRE _{off})	LH ₂ , NH ₃	SC3	t steel	37.58 (2030) 35.23 (2050)	IEA Environmental Projects (2013) for power required + FC efficiency	steel produced x (VRE _{off} (hrs)/24))
Casting (VRE _{off})	LH ₂ , NH ₃	SC3	t steel	0.52 (2030) 0.48 (2050)	IEA Environmental Projects (2013) for power required + FC efficiency	steel produced x (VRE _{off} (hrs)/24))
H₂ or NH₃ for power (JP): $H_{2,annual} (t\ H_2\ or\ NH_3) = demand\ rate\ (kg\ H_2\ or\ NH_3/t) \times quantity\ (t) \times 10^{-3}$						
Applicable processes	Energy vector	SC	Unit	Demand rate (kg H ₂ or NH ₃ /unit)	Source	Qty (annual basis)
H ₂ compression pre-DRI	LH ₂ , NH ₃	SC1	t steel	3.23 kg H ₂ (2030) 3.03 kg H ₂ (2050) 20.82 kg NH ₃ (2030) 19.52 kg NH ₃ (2050)	Aspen Plus Model for power required + FC efficiency	steel produced
EAF	LH ₂ , NH ₃	SC1,2	t steel	37.58 kg H ₂ (2030) 35.23 kg H ₂ (2050) 242.47 kg NH ₃ (2030) 227.32 kg NH ₃ (2050)	Kruger et al. (2020) for power required + FC efficiency	steel produced
Casting	LH ₂ , NH ₃	SC1,2	t steel	0.52 kg H ₂ (2030) 0.48 kg H ₂ (2050) 3.32 kg NH ₃ (2030) 3.11 kg NH ₃ (2050)	IEA Environmental Projects (2013) for power required + FC efficiency	steel produced
H₂ or NH₃ for mobility (JP): $H_{2,annual} (t\ H_2\ or\ NH_3) = demand\ rate\ (t\ H_2\ or\ NH_3/t) \times quantity\ (t)$						
Applicable processes	Energy vector	SC	Unit	Demand rate (kg H ₂ or NH ₃ /unit)	Source	Qty (annual basis)
Dry bulk carrier, Newcastlemax	LH ₂	SC1	Journey (return trip)	250.34 kg H ₂ (2030) 236.43 kg H ₂ (2050)	Refer to shipping fuel consumption calculations	no. journeys
	NH ₃			1479.22 kg NH ₃ (2030)		

Dry bulk carrier, panamax	LH ₂	SC2,3	1397.04 kg NH ₃ (2050)		
	NH ₃		139.90 kg H ₂ (2030) 132.12 kg H ₂ (2050)		
Liquefied gas tanker	LH ₂	SC1,2	826.63 kg NH ₃ (2030) 780.70 kg NH ₃ (2050)		
	NH ₃		289.17 kg H ₂ (2030) 273.11 kg H ₂ (2050) 1708.68 kg NH ₃ (2030) 1613.75 kg NH ₃ (2050)		

Efficiency parameters are summarised in Table S4.6, of which the electrolysis and fuel cell efficiencies have already been applied in the preceding Table S4.5. The symbol (~) indicates no change between 2030 and 2050.

Table S4.6 Process efficiency parameters

Parameter	2030	2050	Applicable processes
Electrolyser efficiency (H ₂ LHV)	68%	75%	- Water electrolysis for H ₂ production
Stationary fuel cell efficiency (H ₂ or NH ₃ LHV)	60%	64%	- Power demands for inflexible processes, following CGH ₂ storage in AU: NH ₃ synthesis, EAF and casting - Power demands in Japan: H ₂ compression pre-DRI, EAF, casting
Mobile fuel cell efficiency (H ₂ or NH ₃ LHV)	68%	72%	- Shipping
Inverter efficiency (electrical)	95%	~	- Between direct VRE DC power supply and AC processes in AU: NH ₃ synthesis, EAF, casting, H ₂ heating pre DRI (AU-VRE _{on}), CGH ₂ storage compression and H ₂ compression pre-DRI. - Between SOFC power supply (following CGH ₂ storage) and AC processes in AU: NH ₃ synthesis, EAF and casting - Between SOFC/PEMFC power supply and electric motors on-board shipping vessels - Between SOFC power supply (following LH ₂ /NH ₃ storage) and AC processes in JP: H ₂ compression pre-DRI, EAF, casting.
Thermal heating efficiency (H ₂ or NH ₃ LHV)	85%	~	- H ₂ heating pre-DRI (AU-VRE _{off} and JP) - NH ₃ cracking
Electrical heating efficiency (electrical)	90%	~	- H ₂ heating pre-DRI (AU-VRE _{on})
LH ₂ shipping efficiency (in terms of BOG mass losses at 0.2%/day)	98.21%	~	- Shipping fuel for liquefied gas tankers - LH ₂ exports, transported in liquefied gas tankers
	97.81%	~	- Shipping fuel for dry bulk carriers
NH ₃ shipping efficiency (in terms of BOG mass losses at 0.02%/day)	99.82%	~	- Shipping fuel for liquefied gas tankers - NH ₃ exports, transported in liquefied gas tankers
	99.78%	~	- Shipping fuel for dry bulk carriers
H ₂ regasification	100%	~	- LH ₂ (at -253°C) or LNH ₃ (at -33°C) utilisation in Japan (considered burden free, enabled by an air exchanger)

Net present value calculations

CAPEX and OPEX were subject to a discount factor:

$$f_d = \frac{1}{(1+i)^N} \quad (\text{Eqn S4.14})$$

where i = real discount rate (%) and N = number of years.

All discounted cash flows over project lifetime were summed to give NPV (\$), then the annualised cost (C_{ann}) calculated:

$$C_{ann, total} (\$/yr) = CRF \times NPV_{total} \quad (\text{Eqn S4.15})$$

$$\text{where Capital Recovery Factor (CRF)} = \frac{i(1+i)^N}{(1+i)^N - 1} \quad (\text{Eqn S4.16})$$

LCOS for one tonne of semi-finished steel was determined by:

$$LCOS (\$/t) = C_{ann, total} \div S \quad (\text{Eqn S4.17})$$

where S = annual steel production (t)

LCOH_p costs could similarly be derived:

$$LCOH_p (\$/kg) = C_{ann, Hp} \div H_p \quad (\text{Eqn S4.18})$$

where $C_{ann, Hp} = CRF \times NPV_{Hp}$, H_p = annual hydrogen production (kg) and NPV_{Hp} = discounted cash flows from relevant CAPEX (electrolyser) and OPEX (electricity, water, labour)

Charter rate calculations

Charter rates were determined based on the vessel, propulsion system and fuel storage CAPEX plus the OPEX of crew, port fees, consumables, maintenance, repair, and insurance.

$$C_{bulk carrier} (\$/day) = (CAPEX + (OPEX \times l)) \div (l \times d) \quad (\text{Eqn S4.19})$$

where:

CAPEX = capital expenditure (\$), including vessel, fuel cell, electric motor, and fuel storage costs (various sources, data in Table S4.8), plus a total investment cost of 10%

OPEX = operational expenditure (\$/year), extracted from (Delhay et al., 2010)

l = lifetime (years), taken as 25 years (Kretschmann et al., 2017)

d = days spent at sea (days/year)

$$C_{gas tanker} (\$/day) = (CAPEX + OPEX) \div (lifetime \times d) \quad (\text{Eqn S4.20})$$

where:

CAPEX (inc. investment cost), OPEX and lifetime are given by Al-Breiki and Bicer (2020a), d = days spent at sea (days/year)

Bulk carrier costs were differentiated by fuel cell improvements between 2030 and 2050. In the absence of better data, the liquefied gas tanker CAPEX was based on a vessel with ICE propulsion system and bunker fuel storage. To account for the cost reductions as a function of FC improvements, a 5% cost reduction was applied for 2050.

Total cost of charter was then determined by:

$$C_{shipping, charter} (\$/year) = c \times V \times d \quad (\text{Eqn S4.21})$$

where: c = charter rate (\$/day), V = number of vessels in fleet, and d = days spent at sea (days/year)

Infrastructure lifetimes

Based on lifetimes, stationary FCs operating in Australia (during VRE_{off}) required replacement every 16-18 years (2030-2050) whilst those operating in Japan (24-hour operation) were replaced every 10-11 years. Mobile FCs were replaced every 5-6 years which formed part of the shipping charter costs. All FC replacements accounted for 33% of initial investment cost (Taljegard et al., 2014).

Apart from FCs, no other infrastructure had to be replaced within the 20-year project lifetime. Solar panels pertained a service life of 25 years (Poulek et al., 2012), CGH_2 , LH_2 and NH_3 plant had a lifetime of 40 years (Bruce et al., 2018) and the DRI-EAF plant had a lifetime of 20 years (Vogl et al., 2018). The alkaline electrolyser lifetime was 95,000 hours in 2030 and 120,000 hours in 2050 (IEA, 2019), and since they operated dynamically during VRE_{on} , this equated to 29 years and 38 years of operation in 2030 and 2050, respectively.

Labour costs

The labour cost was determined as a function of full time equivalent (FTE) employees, which is summarised in Table S4.7.

Table S4.7 Labour-demanding processes and corresponding rates

Process	Rate	Unit	Reference
Electrolysis	0.08	FTE/t H_2 per day	U.S. Department of Energy (DOE) (2012)
DRI	73	FTE/Mt DRI per year	Wood et al. (2020)
EAF	167	FTE/Mt steel per year	
Casting	100	FTE/Mt steel per year	
NH_3 synthesis (exc. electrolysis)	68	FTE/Mt NH_3 per year	
H_2 liquefaction (exc. electrolysis)	386	FTE/Mt H_2 per year	Assumed equivalent to NH_3 synthesis per H_2 output
H_2 compression to 150 bar (exc. electrolysis)	129	FTE/Mt H_2 per year	Assumed 33% of H_2 liquefaction
NH_3 cracking	34	FTE/Mt NH_3 per year	Assumed 50% of NH_3 synthesis

CAPEX and OPEX data

Table S4.8 details CAPEX and OPEX data in 2030 and 2050. Consistently across all plant, maintenance OPEX is taken as 2% of CAPEX. Land purchase costs are not included. The symbol (~) denotes no change in cost within the time interval as the technology is already commercialised.

Table S4.8 CAPEX and OPEX data

	Cost item	2030	2050	Unit	Reference
CAPEX	VRE system (HomerPro inputs)				
	Solar PV	\$ 779	\$ 513	A\$/kW	Graham et al. (2020)
	Wind	\$ 1,812	\$ 1,656	A\$/kW	Graham et al. (2020)
	Grid (90% renewable)	\$ 125	\$ 125	A\$/MWh	Lu et al. (2017)
	Infrastructure, H2-iron-steel plant				
	DRI shaft furnace	\$ 371	~	A\$/Mt DRI capacity	Vogl et al. (2018)
	EAF	\$ 297	~	A\$/Mt steel capacity	Vogl et al. (2018)
	Continuous caster	\$ 68	~	A\$/Mt steel capacity	IEA Environmental Projects (2013)
	Alkaline electrolyser	\$ 884	\$ 637	A\$/kW	IEA (2019)
	CGH2 compressor + vessel	\$ 1,065	~	A\$/kg H2/day	Bruce et al. (2018)
	LH2 liquefier + vessel	\$ 8	~	A\$/kg H2/yr	Bruce et al. (2018)
	NH3 synthesiser + vessel)	\$ 1	~	A\$/kg NH3/yr	Bruce et al. (2018)
	NH3 cracker	\$ 85	~	A\$/kg NH3/day	Institute for Sustainable Process Technology (2017)
	SOFC stack - stationary	\$ 623	\$ 298	A\$/kW	Whiston et al. (2019)
	Shipping				
	SOFC stack - mobile	\$ 623	\$ 298	A\$/kW	Whiston et al. (2019)
	PEMFC stack - mobile	\$ 117	\$ 88	A\$/kW	Marcinkoski et al. (2019)
	Electric motor	\$ 397	~	A\$/kW	de Vries (2019)
	LH2 storage	\$ 339	\$ 241	A\$/GJ	Taljegard et al. (2014)
	NH3 storage	\$ 89	~	A\$/GJ	Korberg et al. (2021)
	Capesize vessel, excluding propulsion system	\$ 34,355	~	A\$ thousands/ship	Compass Maritime Services (2021) reduced by 50% for propulsion system and fuel storage
	Panamax vessel, excluding propulsion system	\$ 20,209	~	A\$ thousands/ship	Compass Maritime Services (2021) reduced by 50% for propulsion system and fuel storage
OPEX	Australian operations				
	Iron ore (2020 average)	\$ 149	~	A\$/t	World Bank Group (2021)
	Labour	\$ 110,476	~	A\$/FTE/yr	2019 mean national wage (OECD, 2021) escalated by 30% for steel industry (Wood et al. 2020)
	Water	\$ 3	~	A\$/kL	International Water Association (2018)
	Japanese operations				
	Labour	\$ 78,423	~	A\$/FTE/yr	2019 mean national wage (OECD, 2021) using OECD exchange rate of 0.65USD/AUD escalated by 30% for steel industry (Wood et al. 2020)
	Water	\$ 1	~	A\$/kL	International Water Association (2018)
	LCOE				
	SC1-LH2	\$ 57	\$ 37	A\$/MWh	HomerPro output
	SC2-LH2	\$ 58	\$ 38	A\$/MWh	HomerPro output
	SC3-LH2	\$ 59	\$ 39	A\$/MWh	HomerPro output
	SC1-NH3	\$ 60	\$ 39	A\$/MWh	HomerPro output
	SC2-NH3	\$ 60	\$ 39	A\$/MWh	HomerPro output
	SC3-NH3	\$ 59	\$ 39	A\$/MWh	HomerPro output
	Charter rates				
	Capesize, LH2-PEMFC	\$ 26,711	\$ 25,880	A\$/day	Calculated from shipping CAPEX and OPEX from Delhay et al., (2010)
	Capesize, NH3-SOFC	\$ 29,904	\$ 26,775	A\$/day	Calculated from shipping CAPEX and OPEX from Delhay et al., (2010)
	Panamax, LH2-PEMFC	\$ 20,144	\$ 19,682	A\$/day	Calculated from shipping CAPEX and OPEX from Delhay et al., (2010)
	Panamax, NH3-SOFC	\$ 21,895	\$ 20,171	A\$/day	Calculated from shipping CAPEX and OPEX from Delhay et al., (2010)
	LH2 tanker	\$ 81,349	\$ 77,282	A\$/day	Calculated from Al-Breiki & Bicer (2020a)
	NH3 tanker	\$ 62,664	\$ 59,531	A\$/day	Calculated from Al-Breiki & Bicer (2020a)

A.ii.2 Supplementary Results

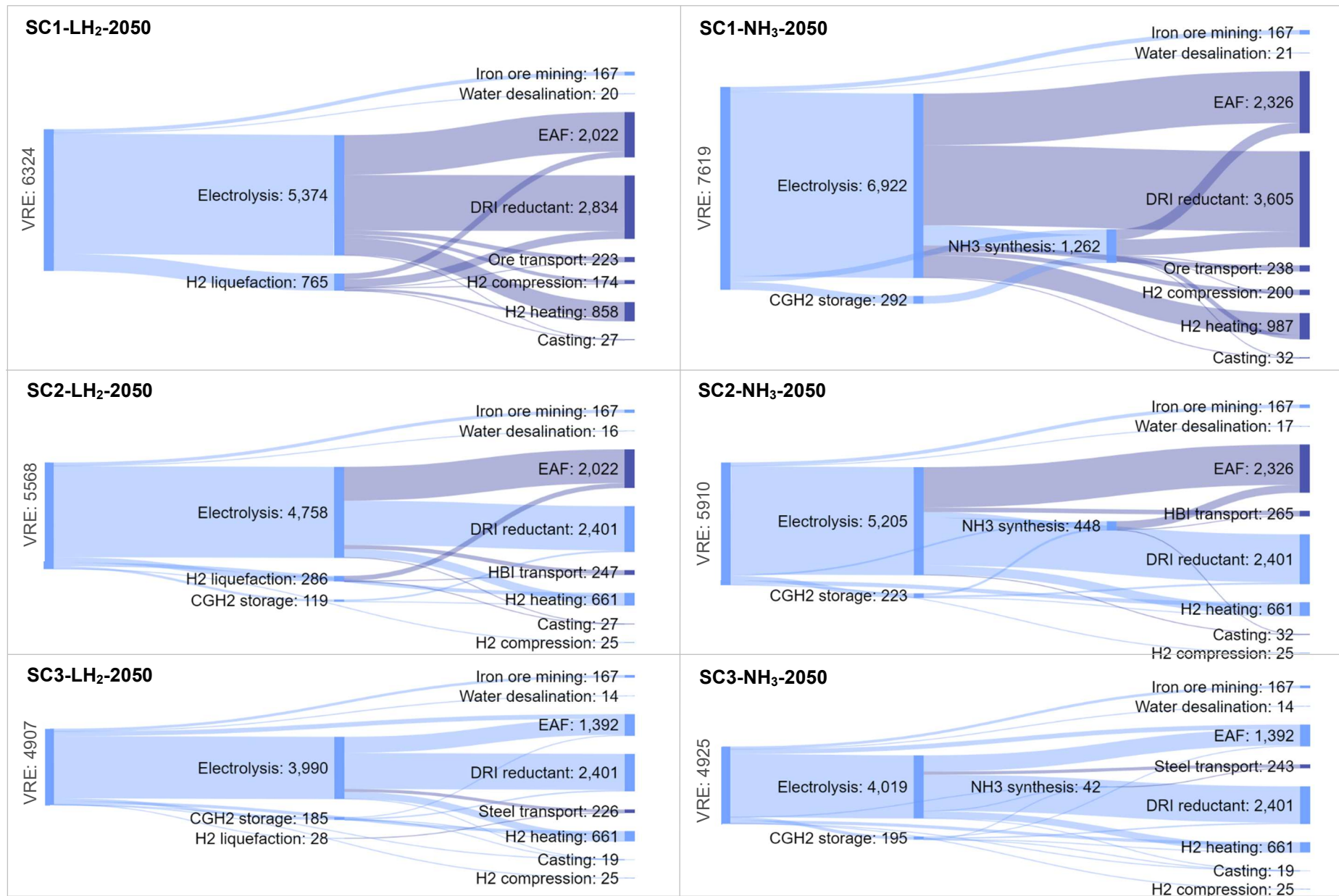


Figure S4.2 Sankey energy distribution diagrams for 2050 cases.

Note: data in kWh/t steel; may not sum due to rounding to nearest whole number; node width correlates to magnitude of energy demand; scale is normalised for all cases.

Shipping fleets and fuel consumption

Results from equations S4.8 to S4.11, regarding shipping vessel journeys, fleets, and departure frequency, are summarised in the table below.

Table S4.9 Vessel fleet logistics

	Export	Vessel	Journeys (no./year)	Duration, one way (days)	Vessels in fleet (no.)	Departure frequency (days)
SC1	Iron ore	Dry bulk, Capesize	361	11	26	1.0
	LH ₂ - 2030	LH ₂ tanker	442	9	27	0.8
	LH ₂ - 2050		431		27	0.8
	NH ₃ - 2030	NH ₃ tanker	306	9	19	1.2
	NH ₃ - 2050		299		18	1.2
SC2	HBI	Dry bulk, Panamax	717	12	53	0.5
	LH ₂ - 2030	LH ₂ tanker	159	9	10	2.3
	LH ₂ - 2050		149		9	2.4
	NH ₃ - 2030	NH ₃ tanker	105	9	7	3.5
	NH ₃ - 2050		98		6	3.7
SC3	Semi-finished steel	Dry bulk, Panamax	656	12	49	0.6

Results from Equation S4.12 and S4.13 for H₂/NH₃ shipping fuel energy demand are summarised in Table S4.10.

Table S4.10 Shipping fuel energy demand (excluding H₂ liquefaction and NH₃ synthesis).

	Shipping fuel energy demand (MWh/t steel)	
	Energy transport (LH ₂ /NH ₃)	Material transport (ore/HBI/steel)
SC1 - LH ₂ - 2030	321	228
SC2 - LH ₂ - 2030	116	253
SC3 - LH ₂ - 2030	-	231
SC1 - LH ₂ - 2050	268	195
SC2 - LH ₂ - 2050	93	216
SC3 - LH ₂ - 2050	-	198
SC1 - NH ₃ - 2030	227	233
SC2 - NH ₃ - 2030	78	258
SC3 - NH ₃ - 2030	-	236
SC1 - NH ₃ - 2050	190	199
SC2 - NH ₃ - 2050	63	221
SC3 - NH ₃ - 2050	-	202

Homer Pro modelling

The 100% VRE system modelled through Homer Pro was completed using the deferrable load module with key inputs, and subsequent results, detailed in Table B.3.

Table S4.11 Homer Pro data inputs and results

	Inputs				Results		
	Daily load (kWh/d)	Peak load (kW)	Storage capacity (kWh)	storage capacity/daily load	LCOE (A\$/MWh)	CAPEX (A\$ millions)	Solar capacity (MW)
SC1 - LH ₂ - 2030	807,833,595	89,759,288	807,833,595	100%	57.27	149,951	192,492
SC2 - LH ₂ - 2030	681,333,201	75,703,689	553,052,631	81%	58.14	128,543	165,010
SC3 - LH ₂ - 2030	572,537,710	63,615,301	411,468,351	72%	58.77	109,179	140,152
SC1 - LH ₂ - 2050	669,046,045	74,338,449	669,046,045	100%	37.41	81,560	158,986
SC2 - LH ₂ - 2050	586,984,653	65,220,517	468,426,815	80%	38.02	72,732	141,778
SC3 - LH ₂ - 2050	515,157,444	57,239,716	363,810,818	71%	38.55	64,693	126,106
SC1 - NH ₃ - 2030	918,102,580	102,011,398	608,227,579	66%	60.01	178,800	229,526
SC2 - NH ₃ - 2030	706,373,129	78,485,903	463,712,148	66%	59.96	137,566	176,593
SC3 - NH ₃ - 2030	572,980,001	63,664,445	401,423,595	70%	59.06	109,844	141,007
SC1 - NH ₃ - 2050	810,044,473	90,004,941	534,227,283	66%	39.26	103,888	202,511
SC2 - NH ₃ - 2050	624,212,585	69,356,954	407,740,505	65%	39.27	80,055	156,053
SC3 - NH ₃ - 2050	517,084,091	57,453,788	356,686,042	69%	38.73	65,280	127,251

Water and land footprints

Water footprint was assessed, considering both Australia- and Japan-based production. As shown in Table B.4, most of the water demand was for supplying cooling water, where water consumed was a fraction of the water withdrawn. Two return “loops” were considered for water re-use; water consumed for electrolysis at the same rate of release from (i) DRI or (ii) fuel cell power generation (assuming continuous operation with no H₂ losses). The resultant water consumption reduction is only attained if both processes occur in the same location:

- SC2 and SC3: H₂ production (electrolysis) and DRI in Australia
- All excluding LH₂-SC1: H₂ production (electrolysis) and H₂ consumption for power generation in Australia

Table S4.12 Water-consuming production processes

Process	Type	Unit	L/unit			Reference
			Withdrawn	Returned	Consumed	
VRE production	Cleaning water	MWh	42	0	42	(Jin et al., 2019)
Water electrolysis	Process water	kg H ₂	9	0	9	Stoichiometry
DRI	Return water	kg H ₂	0	8.55	-8.55	Stoichiometry (+5% losses)
Fuel cell power generation	Return water	kg H ₂	0	8.55	-8.55	Stoichiometry (+5% losses)
EHF	Cooling water	t LS	28100	26500	1600	(worldsteel, 2020c)
Casting	Cooling water	t LS	n/a	n/a	1000	(IEAGHG, 2013)

Land footprint was quantified for Australia-based production only, due to the dominating spatial factor of solar panels, for which the solar power capacity was determined through Homer Pro modelling. Table B.5 details the land consumption rates for key infrastructure components, including energy storage

tanks as energy storage is an potentially important spatial consideration varying with the distinct densities of CGH₂ at 150 bar (11 kg/m³), LH₂ (71 kg/m³) and NH₃ (682 kg/m³) (Bruce et al., 2018; Klüssmann et al., 2020). For calculating the footprints of these storage tanks, a 24-hour capacity was used for each storage, which was deemed sufficient considering the primarily diurnal (as opposed to seasonal) intermittency of VRE and high frequency of shipping vessels leaving Port Hedland (approximately 1 vessel per day).

Table S4.13 Land-consuming processes and corresponding rates

Infrastructure	m ² /unit	unit	Reference
Solar PV panels	28,000	MW	Bruce et al. (2018)
Alkaline electrolyzers	95	MW	IEA (2019)
LH ₂ spherical storage tank	2.7	t LH ₂ (24-hr capacity)	van Hoecke et al. (2021)
NH ₃ storage tank	0.017	t NH ₃ (24-hr capacity)	Based on LNG tank, Yang et al. (2006)
CGH ₂ storage tank (150 bar)	18.2	t CGH ₂ (24-hr capacity)	Bruce et al. (2018)

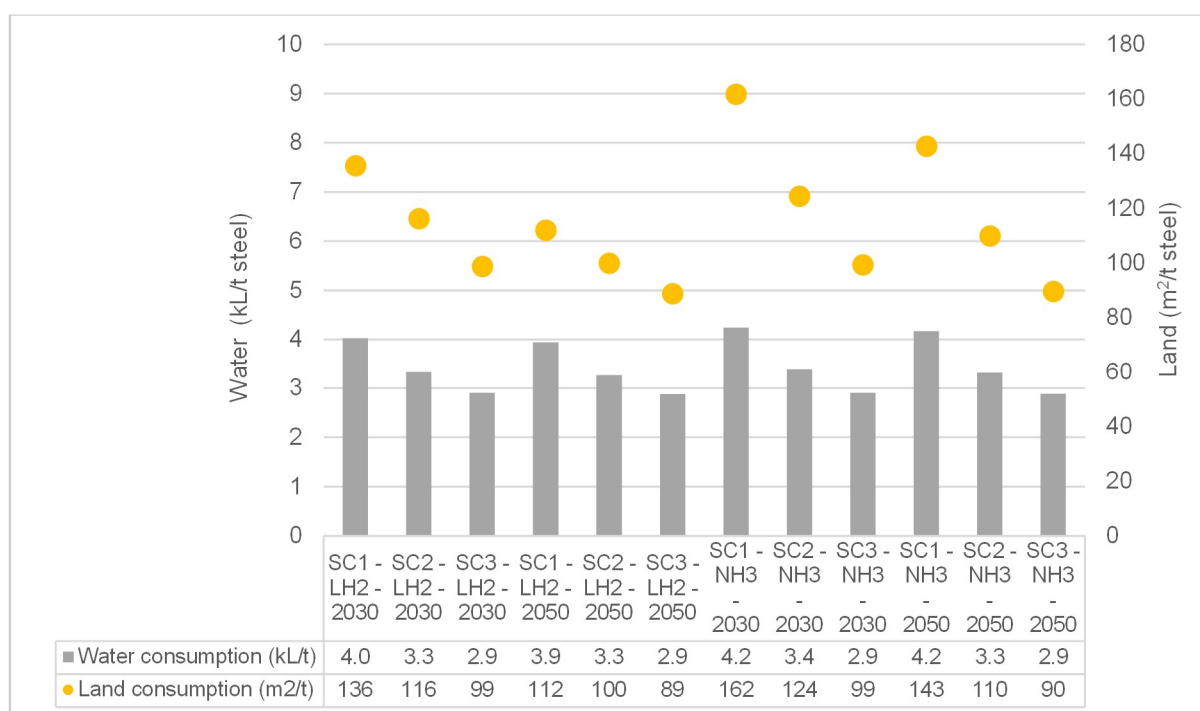


Figure S4.3 Water and land demand, per tonne of semi-finished steel

Sensitivity analysis

A sensitivity analysis of key process efficiencies, all varied $\pm 5\%$ from the base case, was carried out on LH₂-2050 and NH₃-2050 cases. The favourable and unfavourable variable inputs are detailed in Table B.6, with results in Figures B.3 and B.4.

Table S4.14 – Sensitivity analysis variables

			Variable			
Process	Case	Basis	Favourable	Base	Unfavourable	Range
Technology in development						
Electrolyser efficiency - 2050	LH ₂ -2050	% (H ₂ , LHV)	78.8%	75%	71.3%	+/- 5% to the base case
Liquefaction efficiency - 2050	LH ₂ -2050	% (H ₂ , LHV)	86.1%	82%	77.9%	+/- 5% to the base case
FC efficiency - stat - 2050	LH ₂ -2050	% (H ₂ , LHV)	67.2%	64%	60.8%	+/- 5% to the base case
FC efficiency - mobile - 2050	LH ₂ -2050	% (H ₂ , LHV)	75.6%	72%	68.4%	+/- 5% to the base case
Mature technology (requiring breakthrough)						
EAF	LH ₂ -2050	MWh/t LS	0.714	0.752	0.789	+/- 5% to the base case
H ₂ heating pre-DRI	LH ₂ -2050	MWh/t LS	0.424	0.446	0.468	+/- 5% to the base case
NH ₃ synthesis	NH ₃ -2050	MWh/t NH ₃	0.664	0.699	0.734	+/- 5% to the base case
NH ₃ cracking	NH ₃ -2050	kg H ₂ (cracked)/ kg NH ₃ (heat)	9.127	8.692	8.257	+/- 5% to the base case

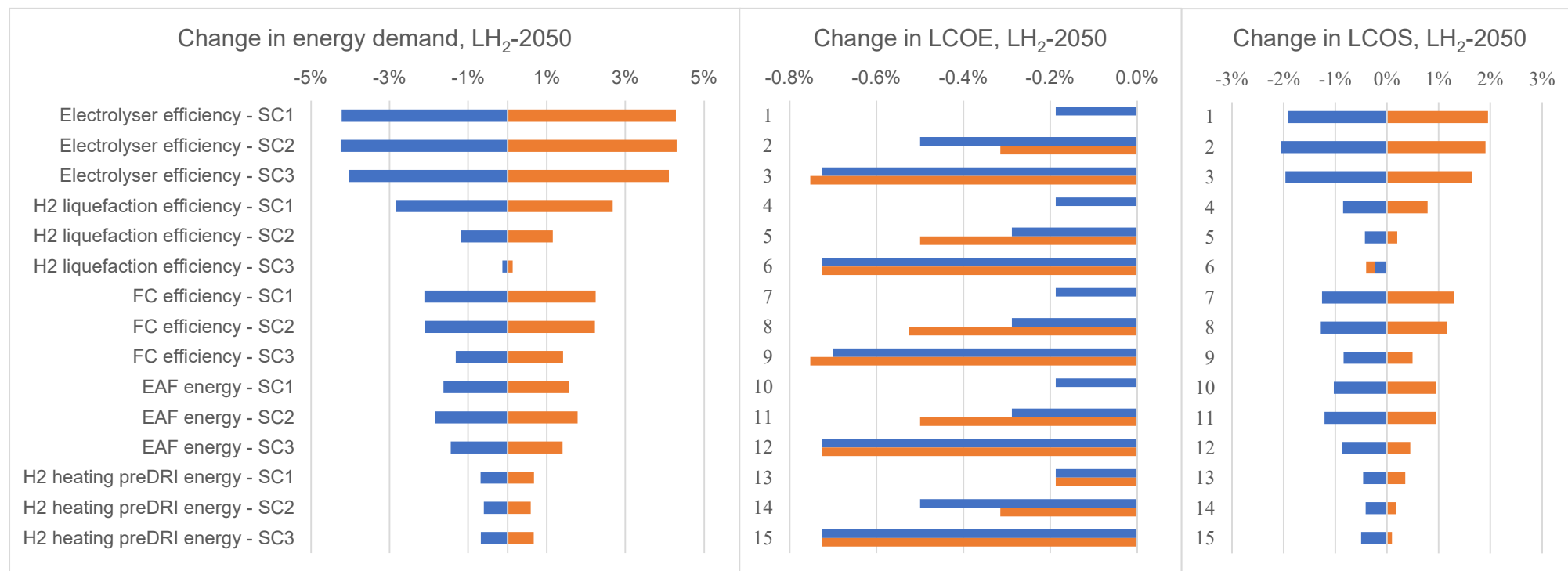


Figure S4.4 LH₂-2050 sensitivity analysis results for (a) change in energy demand, (b) LCOE and (c) LCOS.

■ Favourable ■ Unfavourable

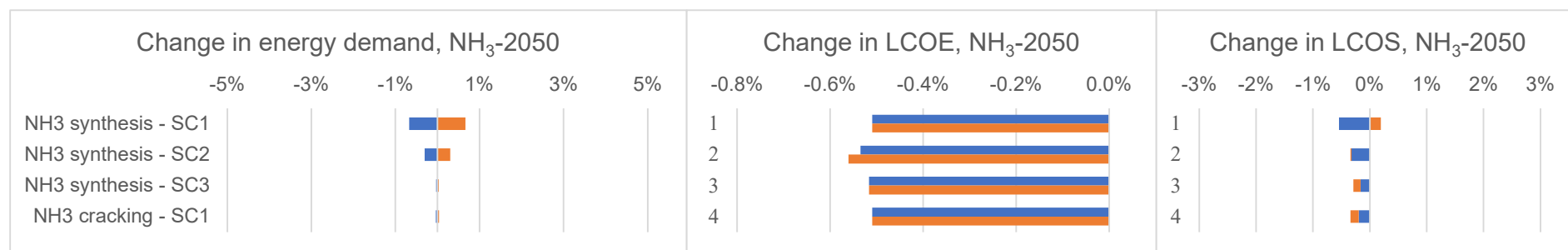


Figure S4.5 NH₃-2050 sensitivity analysis results for (a) change in energy demand, (b) LCOE and (c) LCOS.

Appendix III: Supplementary Information to Chapter 5

A.iii.1 Supplementary Results

Renewable power, hydrogen, and ammonia potential

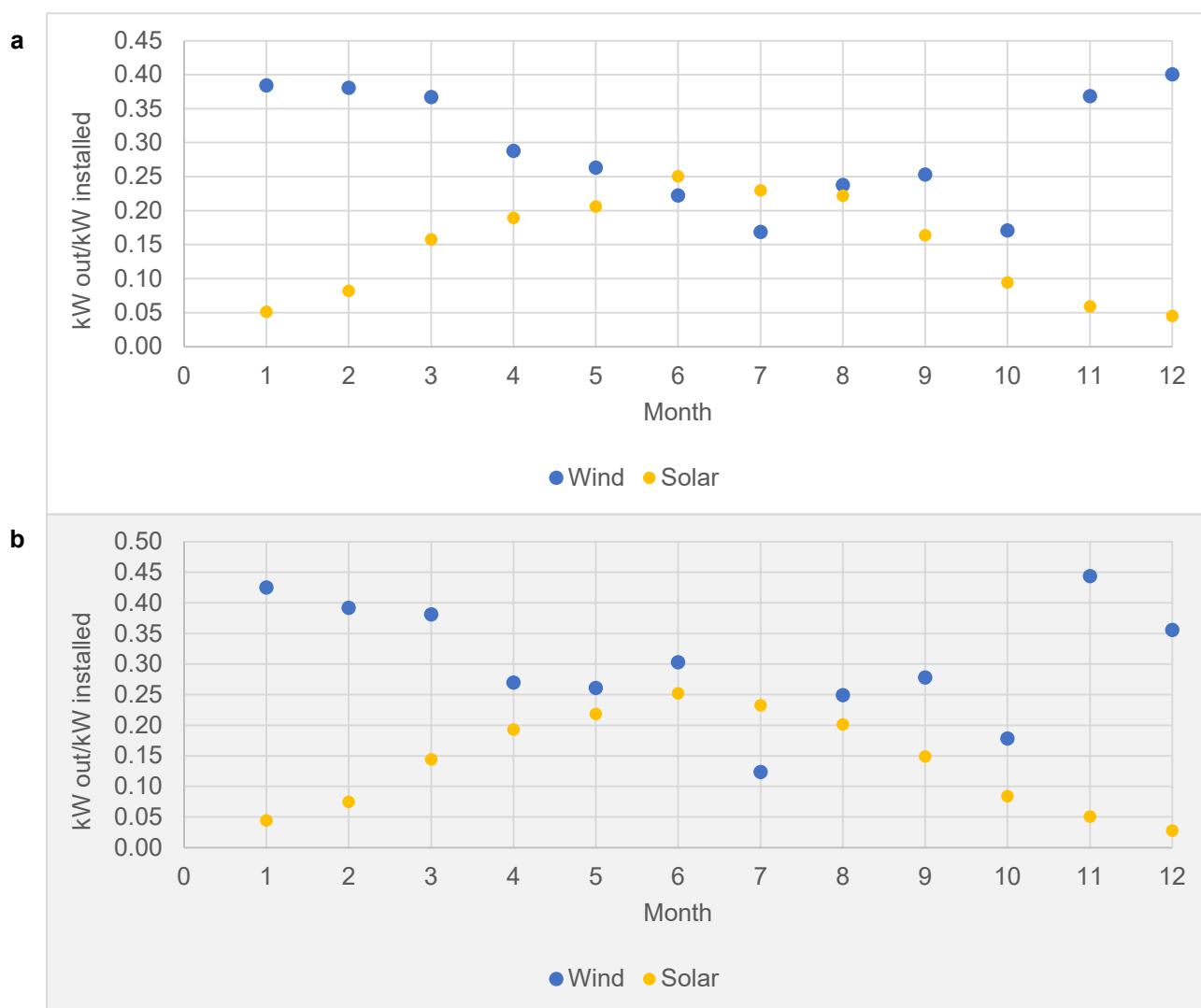


Figure S5.1 Variable renewable energy capacity profiles for each month in 2019 based on analysis of ERA5 climatic data, displayed for two locations – (a) Odesa oblast with coordinates 46°, 29° (grid #s01), (b) Dnipropetrovsk oblast with coordinates 48°. 34° (grid #s18).

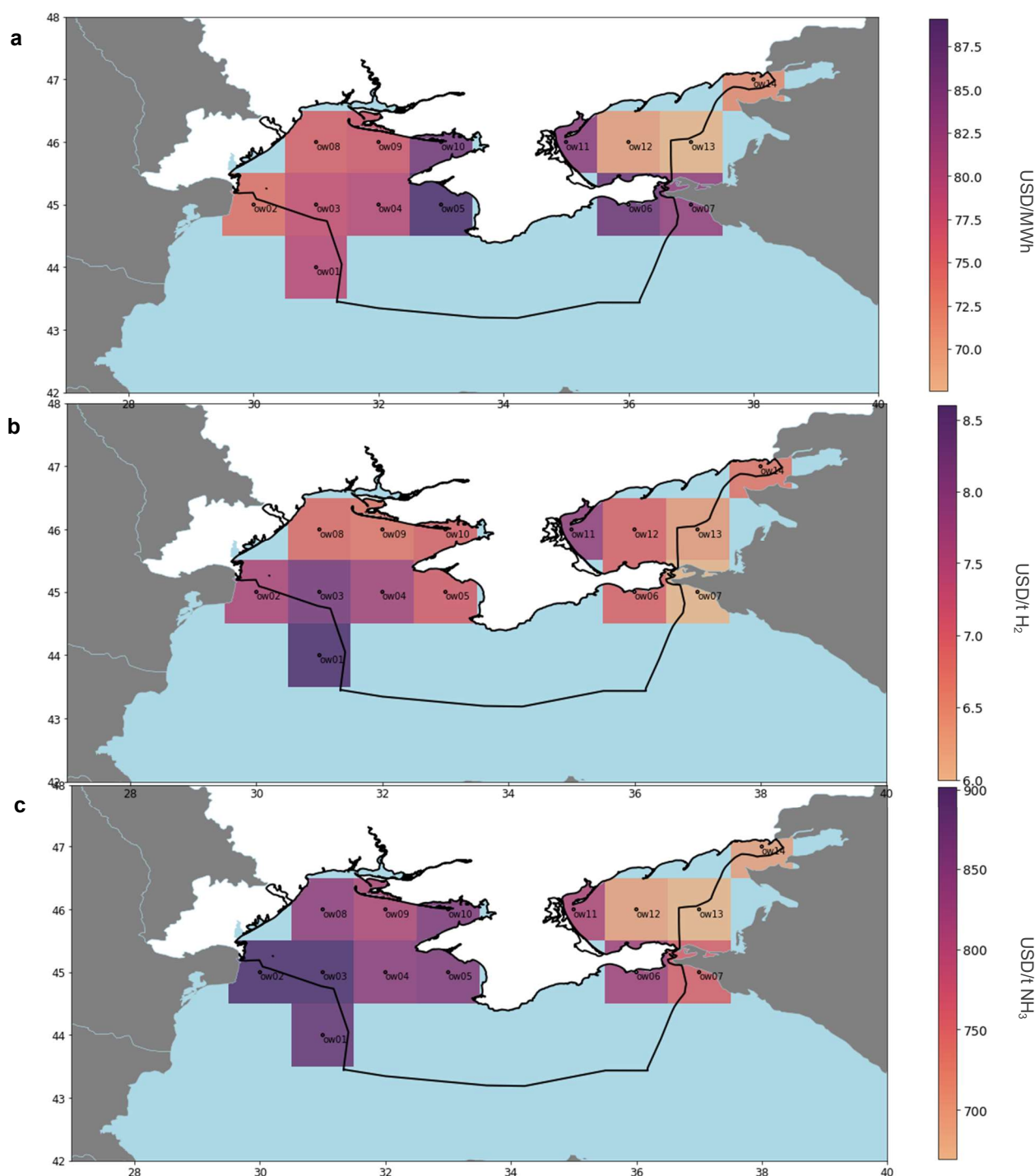


Figure S5.2 Cost-minimised results of offshore wind plant energy products in 2050, at 1°x1° grid spatial resolution, projected on equal axes so that longitude and latitudes are equidistant - (a) Levelised cost of firm electricity (in USD/MWh). (b) Levelised cost of continually supplied hydrogen (in USD/t H₂). (c) Levelised cost of continually supplied ammonia (in USD/t NH₃). Locations with water depths <50m utilise fixed turbines, and <1000m floating turbines - all locations with water depth >1000m are not assessed. Fourteen grids sat at least partially within Ukraine's exclusive marine economic zone within the Black and Azov Seas, and with sea depths less than 1000m. The average levelised cost of offshore wind is \$103, \$89.5 and \$79.4/MWh in 2030, 2040 and 2050, respectively, including substantial CGH₂, NH₃ and battery storage to assure firm power supply. Green fuel costs were similarly steep: \$9.32, \$8.09 and \$7.20/kg H₂, and \$1084, \$931 and \$824/t NH₃, for 2030, 2040 and 2050, respectively.

Green HBI and green steel competitiveness

Prior to investigating optimal production and trade supply chains, steel production costs via different technological routes were assessed to understand the model's technology and fuel selection. For domestic green steel production, the BF-BOF production route is likely to be the cheapest without carbon pricing mechanisms in place, even against low-priced and continuous zero-carbon power from nuclear and/or hydropower. Favourably for industrial decarbonisation, compliance to the EU-ETS or a very similar UA-ETS is considered across all scenarios. In ascending order, the levelised cost of steel (LCOS) for the BF-BOF route was estimated at \$415/t steel, scrap-EAF route at \$472/t steel, NG-DRI-EAF route at \$483/t steel, and H₂-DRI-EAF route at \$621/t steel. Looking at H₂/NG blends for DRI, a 30/70 split led to an LCOS of \$496/t steel, and a 65/35 split led to an LCOS of \$542/t steel. The relative costs of production via different production routes are sensitive to the price of input commodities, especially iron ore (base case of \$100/t for DR-grade, \$80/t for BF-grade), metallurgical coal (base case of \$200/t), natural gas (base case of \$25/MWh), electricity, and hydrogen. Through a sensitivity analysis, it was deduced that a 50% increase in metallurgical coal will increase BF-BOF costs by 14%, a 50% increase in NG price will increase NG-DRI-EAF costs by 7%, a 50% increase in scrap price will increase scrap-EAF costs by 33%, and a 50% increase in RE and H₂ price will increase H₂-DRI-EAF costs by 20%. The levelised costs of steel and sensitivity analyses of various steel production routes are detailed in this section.

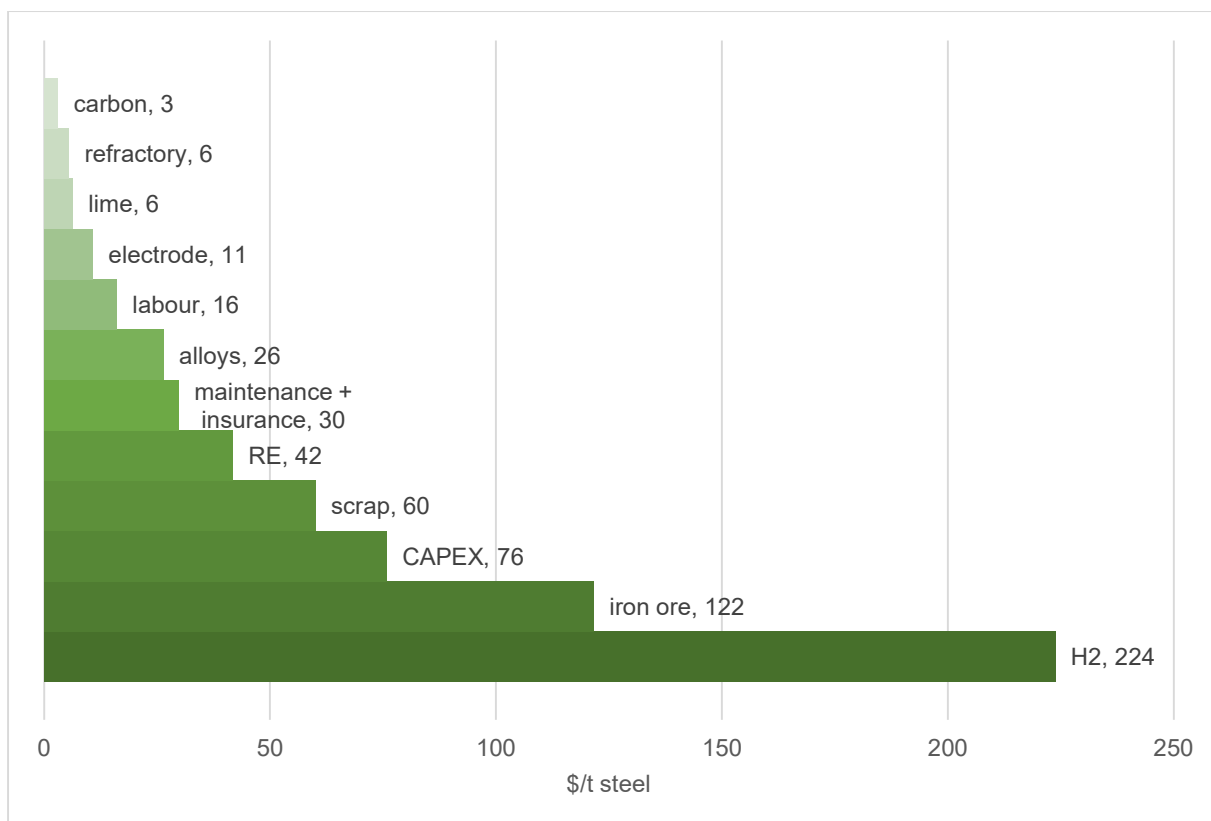


Figure S5.3 Levelised cost of steel breakdown for the H2-DRI-EAF route, totalling \$621/t steel.

Table S5.1 Sensitivity analysis of key commodities within the LCOS of the H2-DRI-EAF route.

	Unit	UA base	S.A. range	Favourable	Un-favourable	LCOS impact
<i>DR-grade ore price</i>	\$/t	100	± 30%	70	130	± 4%
<i>RE price</i>	\$/MWh	70	± 50%	35	105	± 2%
<i>H₂ price</i>	\$/t	3.8	± 50%	1.9	5.75	± 18%
<i>Scrap price</i>	\$/t	300	± 50%	150	450	± 5%
<i>Discount rate</i>	%	8	± 50%	12	4	+4%

The co-located H₂-DRI-EAF results slightly differ our previous study (Devlin et al., 2023) due to different climatic data inputs (this study uses ERA5 instead of MERRA-2). In this study, analysis of hourly ERA5 climatic data (Hersbach, 2023) determined the maximum capacity factor of solar to be 14%, and wind to be 31% for the same location for the year 2019. This aligns with research by the Institute of Renewable Energy (Ukrainian Institute of Renewable Energy, 2020), which determined the capacity factor of solar to be 14% and onshore wind to be 31% (plus offshore wind to be 45%).

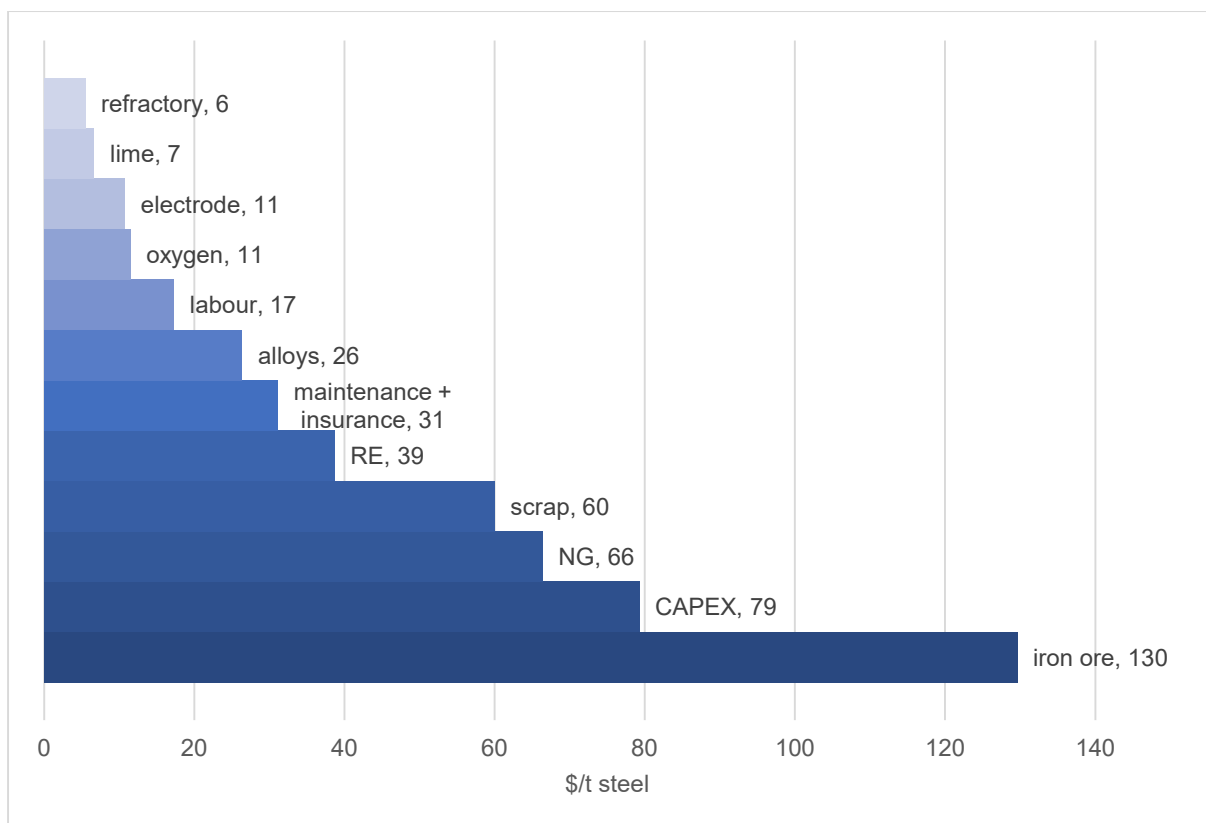


Figure S5.4 Levelised cost of steel breakdown for the NG-DRI-EAF route, totalling \$483/t steel.

Table S5.2 Sensitivity analysis of key commodities within the LCOS of the NG-DRI-EAF route.

	Unit	UA base	S.A. range	Favourable	Un-favourable	LCOS impact
DR-grade ore price	\$/t	100	± 30%	70	130	± 7%
RE price	\$/MWh	70	± 50%	35	105	± 4%
NG price	\$/MWh	25	± 30%	12.5	37.5	± 7%
Scrap price	\$/t	300	± 50%	150	450	± 5%
Discount rate	%	8	± 50%	12	4	+4%

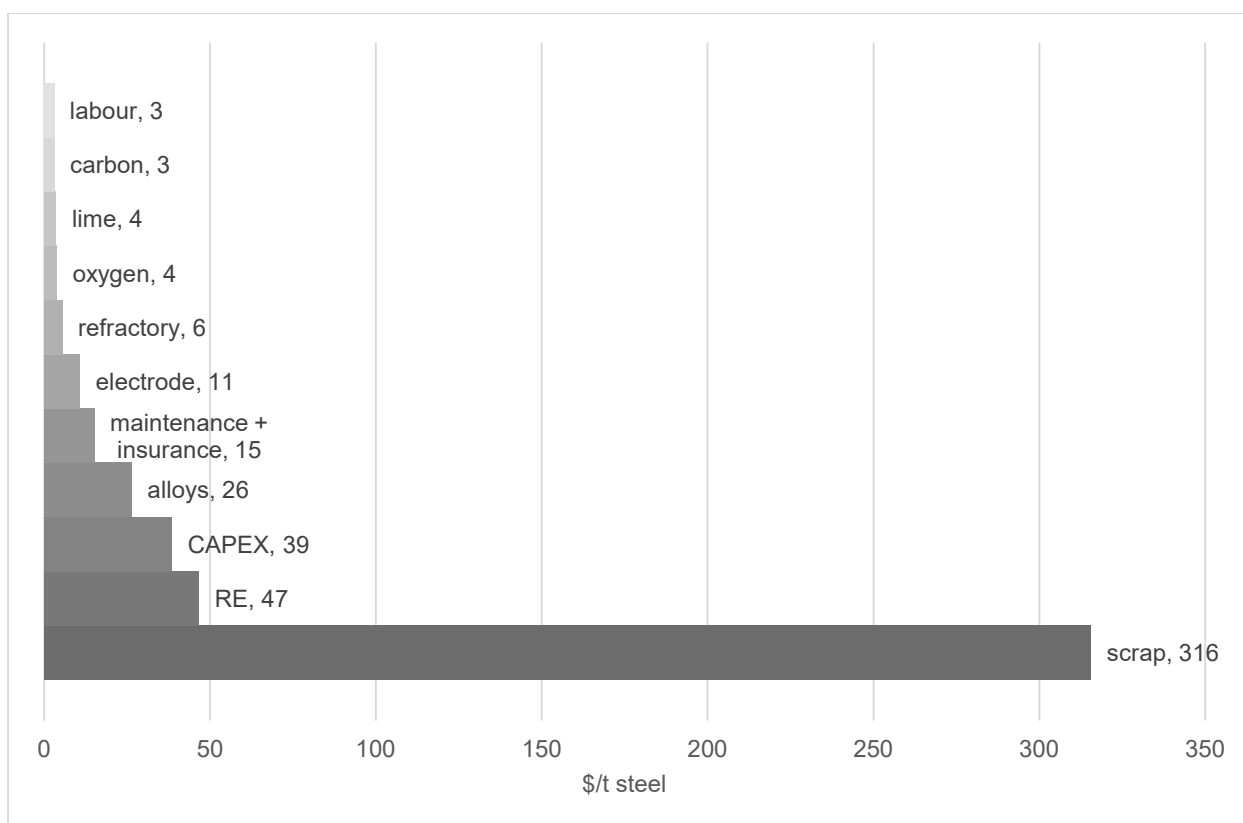


Figure S5.5 Levelised cost of steel breakdown for the scrap-based EAF route, totalling \$472/t steel.

Table S5.3 Sensitivity analysis of key commodities within the LCOS of the scrap-based EAF route.

	Unit	UA base	S.A. range	Favourable	Un-favourable	LCOS impact
RE price	\$/MWh	70	± 50%	35	105	± 5%
Scrap price	\$/t	300	± 50%	150	450	± 33%
Discount rate	%	8	± 50%	12	4	+3%

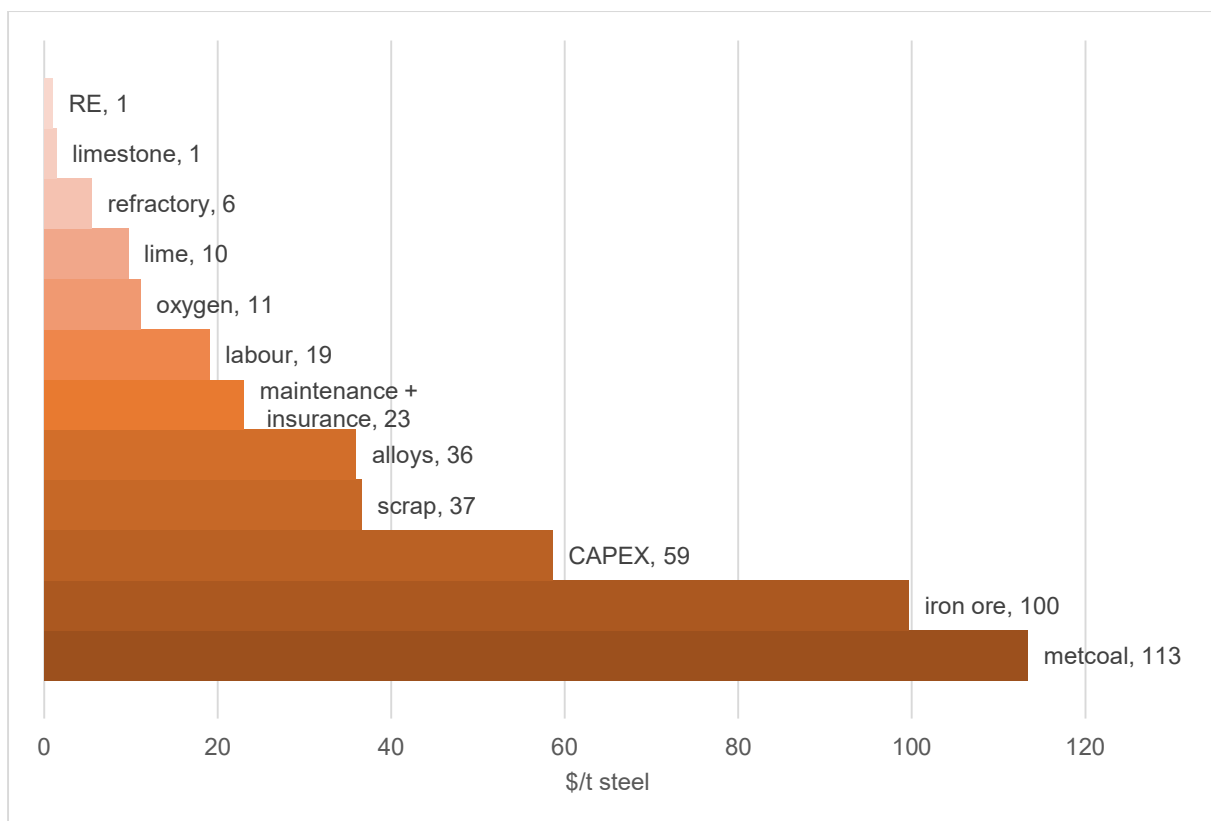


Figure S5.6 Levelised cost of steel breakdown for the BF-BOF route, totalling \$415/t steel.

Table S5.4 Sensitivity analysis of key commodities within the LCOS of the BF-BOF route.

	Unit	UA base	S.A. range	Favourable	Un-favourable	LCOS impact
<i>BF-grade ore price</i>	\$/t	80	± 20%	56	104	± 7%
<i>Met coal price</i>	\$/t	200	± 30%	140	260	± 8%
<i>Scrap price</i>	\$/t	300	± 50%	150	450	± 4%
<i>Discount rate</i>	%	8	± 50%	12	4	+4%

Table S5.5. Levelised cost of iron (LCOI) and levelised cost of steel (LCOS) breakdown for the green H2-DRI-EAF route.

Year	min LCOE (\$/MWh)	min LCOH (\$/t H2)	LCOHBI (\$/t HBI)	80% DRI/20% scrap			100% DRI		
				LCOS (\$/t steel)	Δ (\$/t steel)	HBI costs of steel (%)	LCOS (\$/t steel)	Δ (\$/t steel)	HBI costs of steel (%)
2030	96	5.03	506	653	198	70%	719	162	77%
2040	77	4.01	458	604	192	68%	657	154	77%
2050	64	3.31	441	587	190	68%	636	151	76%

Forecast steel demand and scrap availability

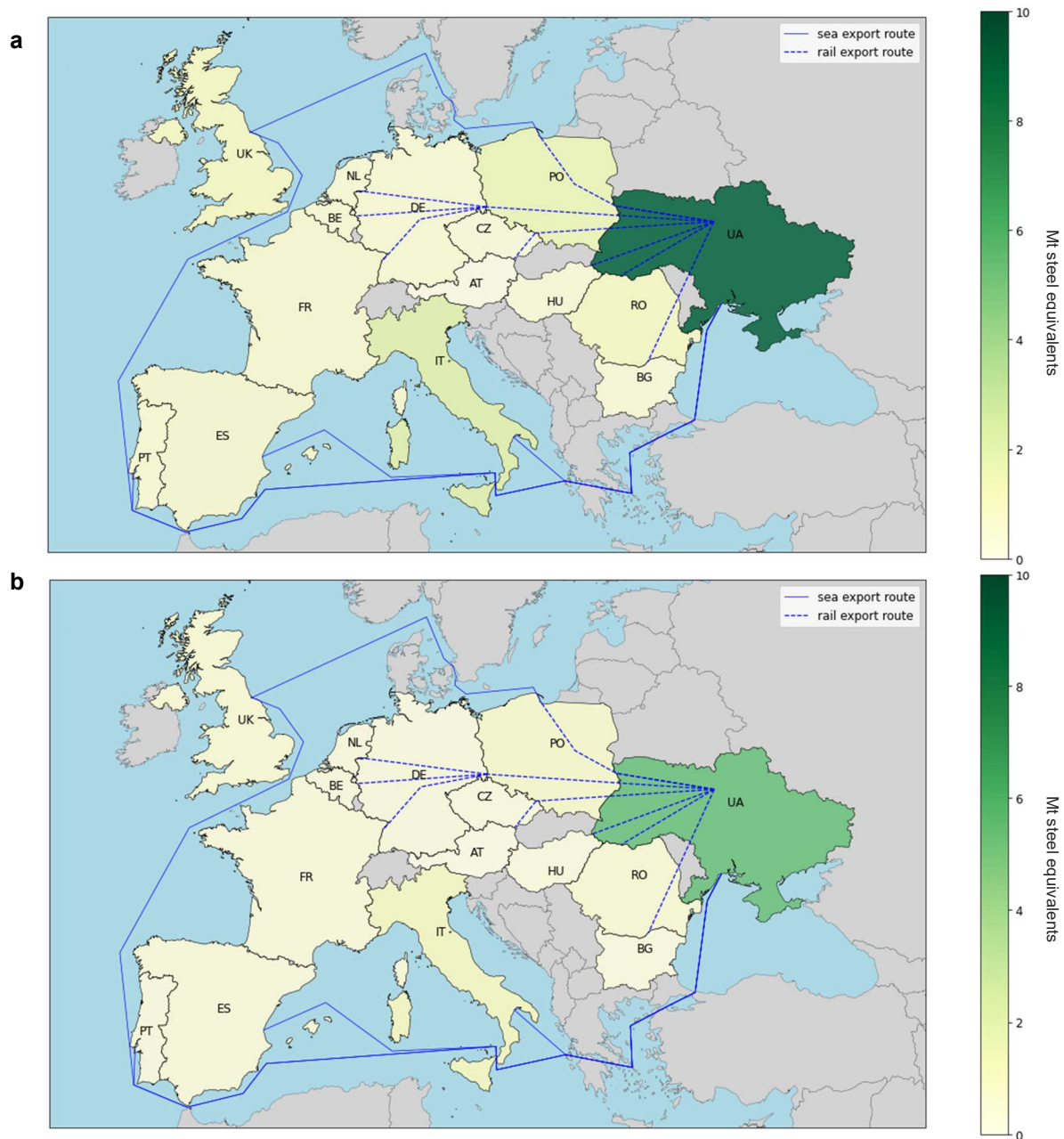


Figure S5.7 Domestic steel demand and steel/HBI export flows in 2030 for the (a) Strong Recovery scenario, and (b) Slow Recovery scenario. HBI and steel exports are compounded as steel equivalents (given 0.9 t HBI/t steel with 14% scrap charge).

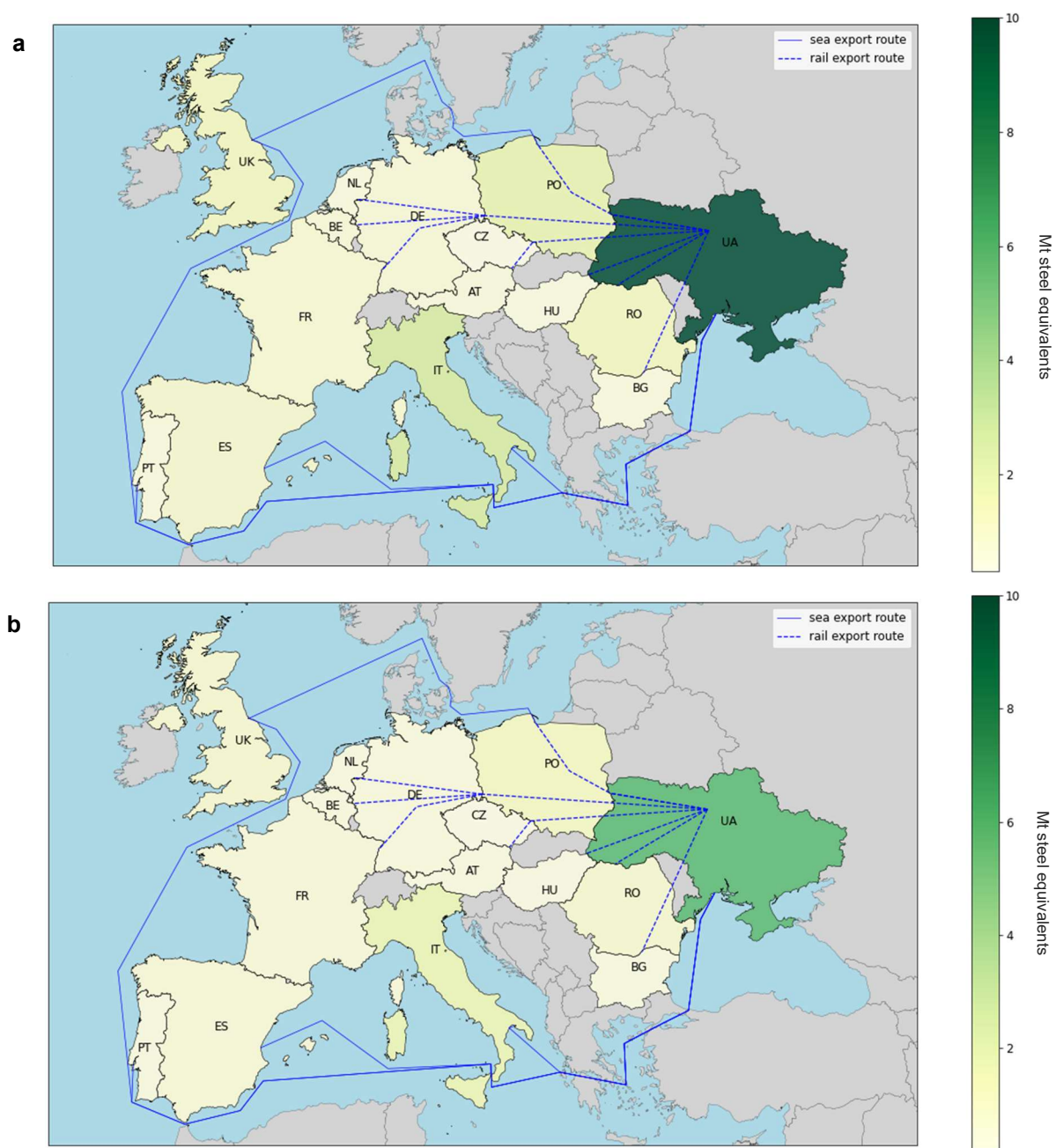


Figure S5.8 Domestic steel demand and steel/HBI export flows in 2040 for the (a) Strong Recovery scenario, and (b) Slow Recovery scenario. HBI and steel exports are compounded as steel equivalents (given 0.9 t HBI/t steel with 14% scrap charge).

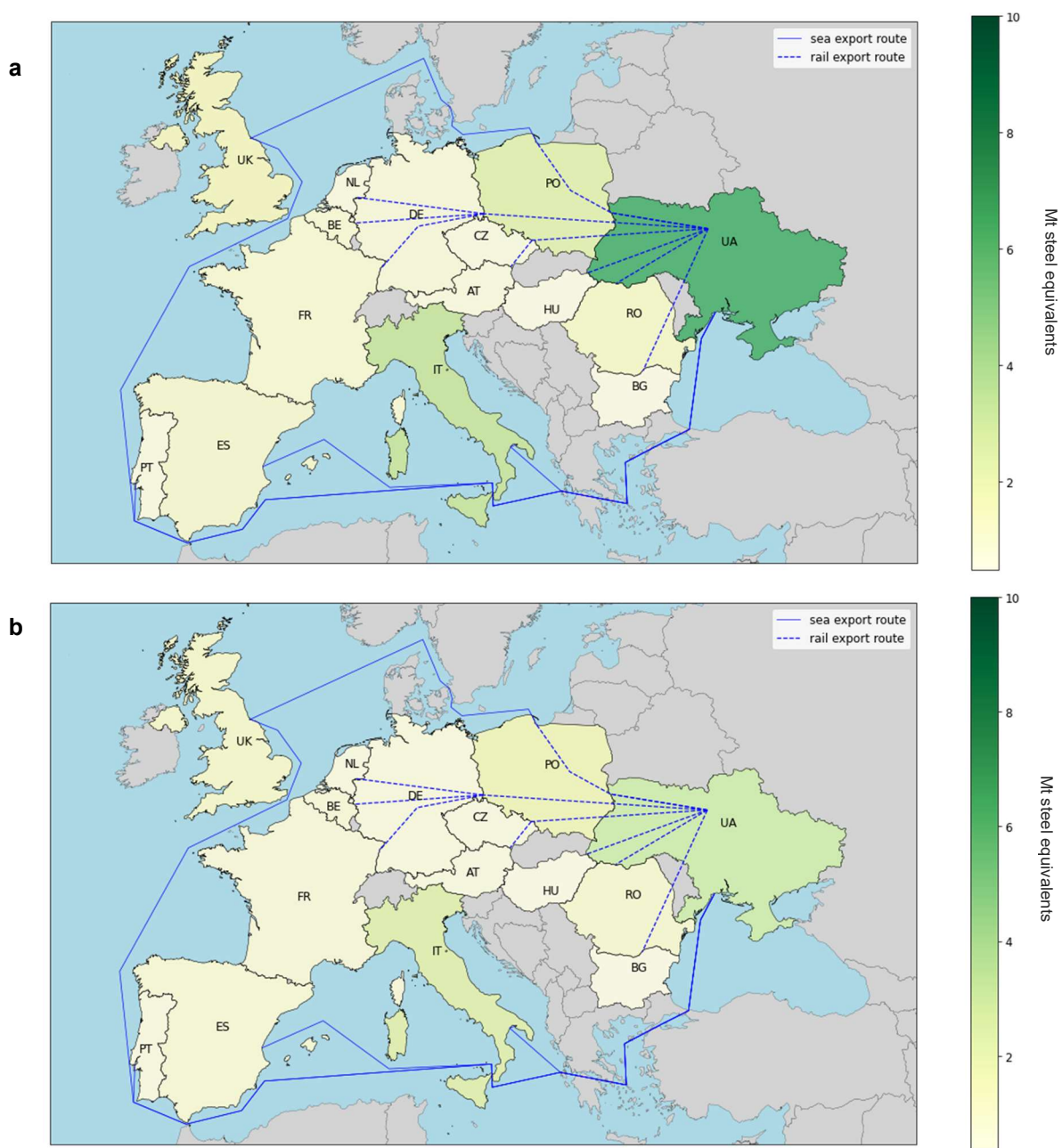


Figure S5.9 Domestic steel demand and steel/HBI export flows in 2050 for the (a) Strong Recovery scenario, and (b) Slow Recovery scenario. HBI and steel exports are compounded as steel equivalents (given 0.9 t HBI/t steel with 14% scrap charge).

Production and trade optimisation

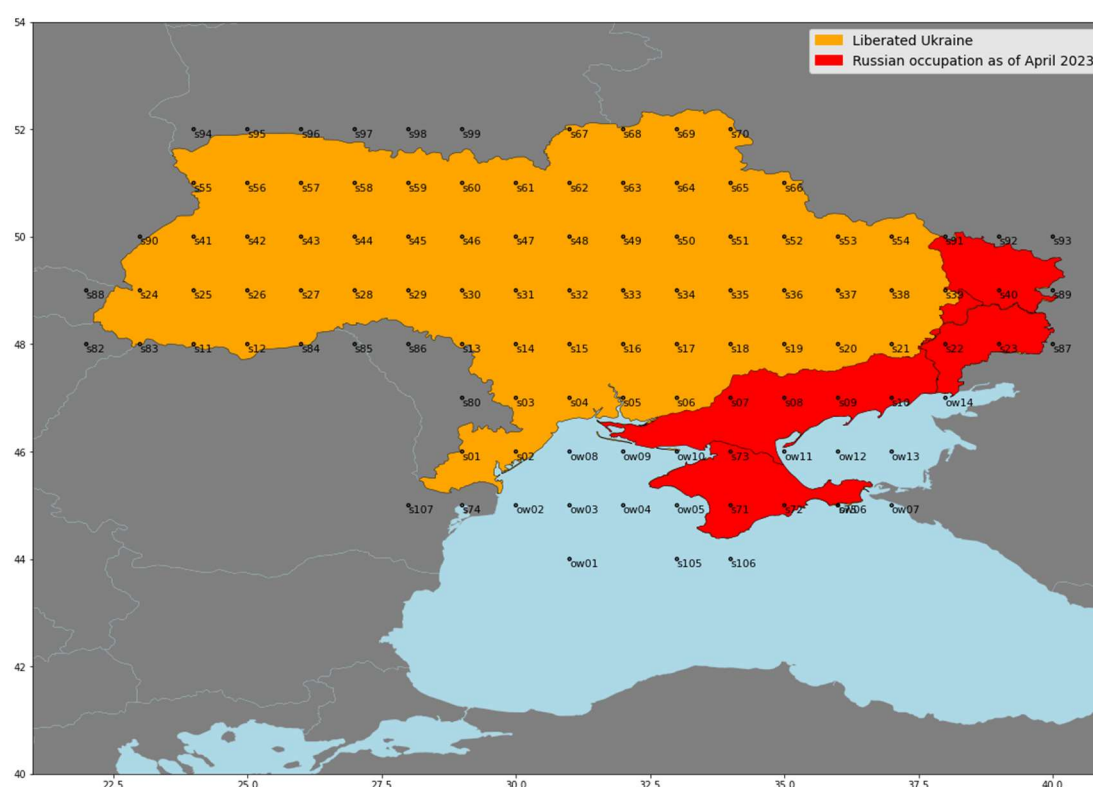


Figure S5.10 Grid identification and location for onshore energy production and manufacturing sites, and offshore wind energy production sites.

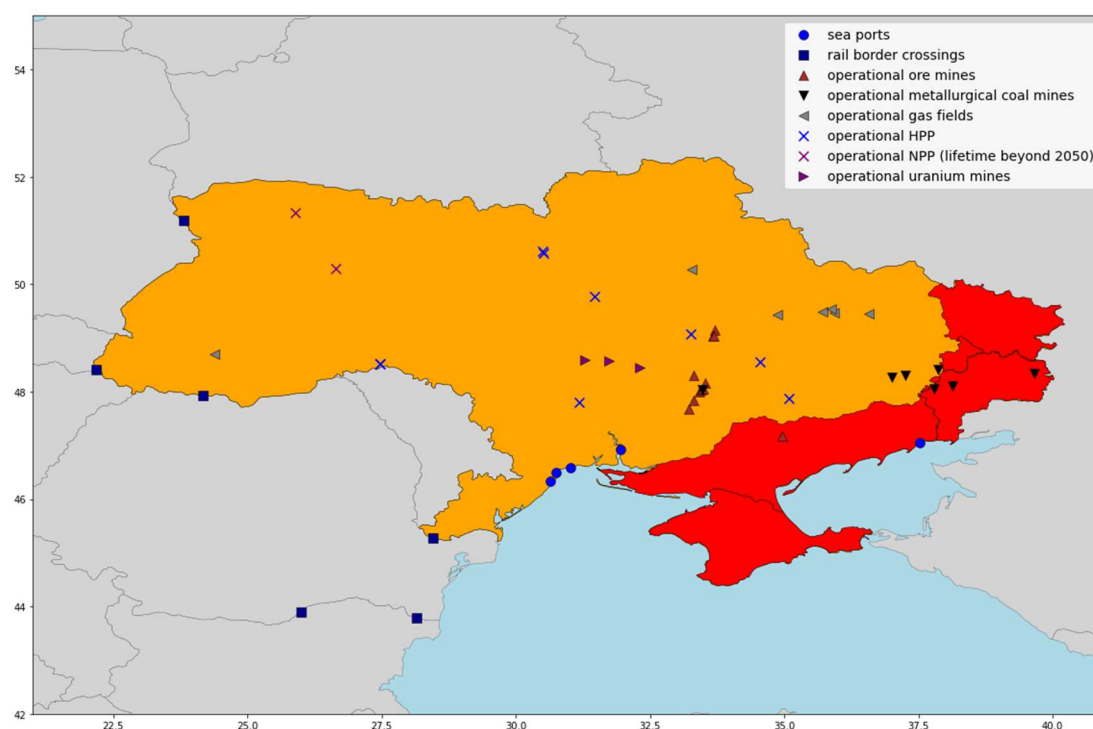


Figure S5.11 Iron and steel supply chain asset map, illustrating the location of relevant mines, established nuclear and hydropower plants, and critical transportation nodes for exports.

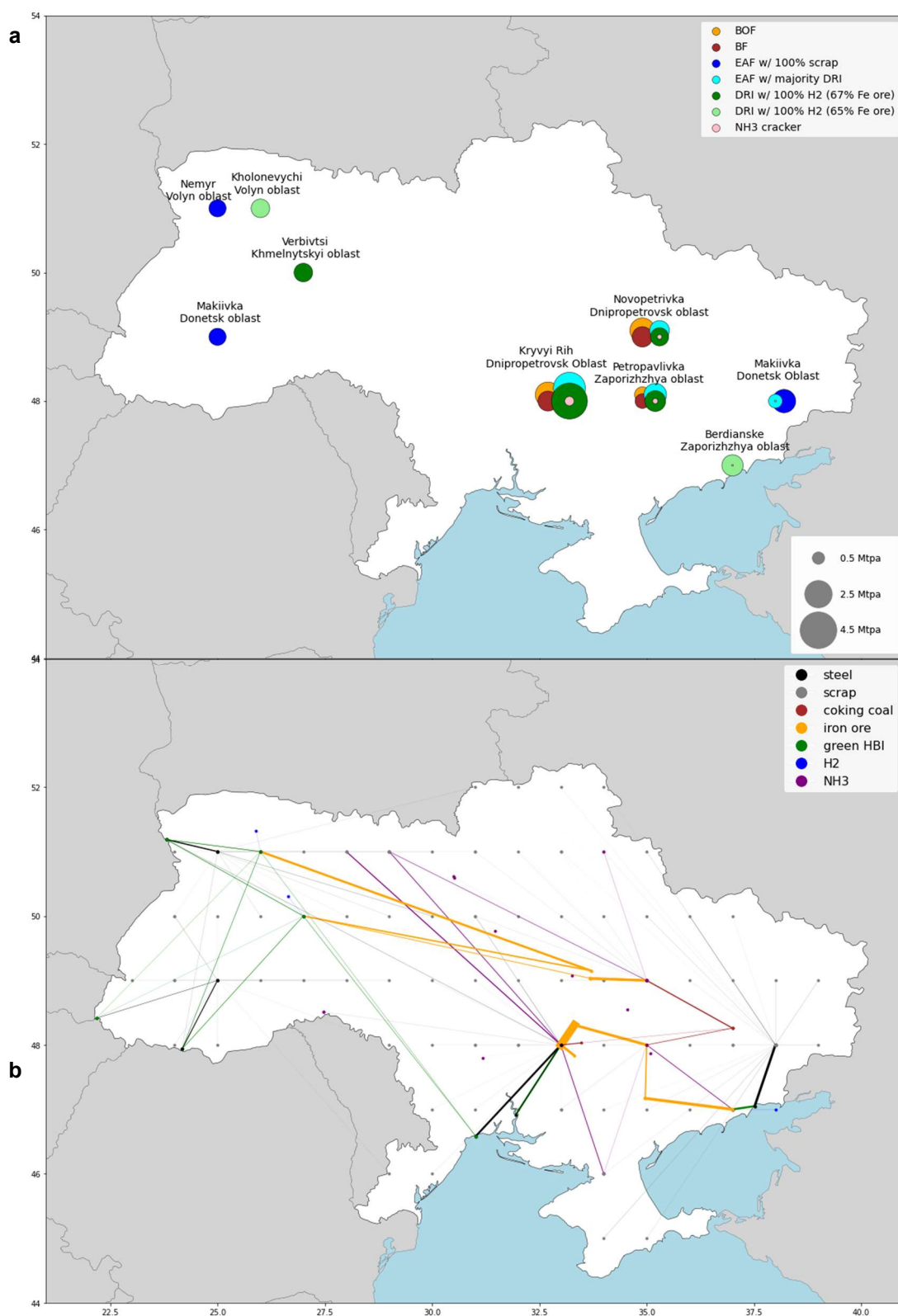


Figure S5.12 Optimised steel supply chains in 2030 under the Full Liberation & Steady Recovery Scenario: (a) capacity of iron and steel production assets (marker diameter indicates rated capacity), and (b) domestic supply chain flows (straight-line distances shown, line thickness indicates trade volume).

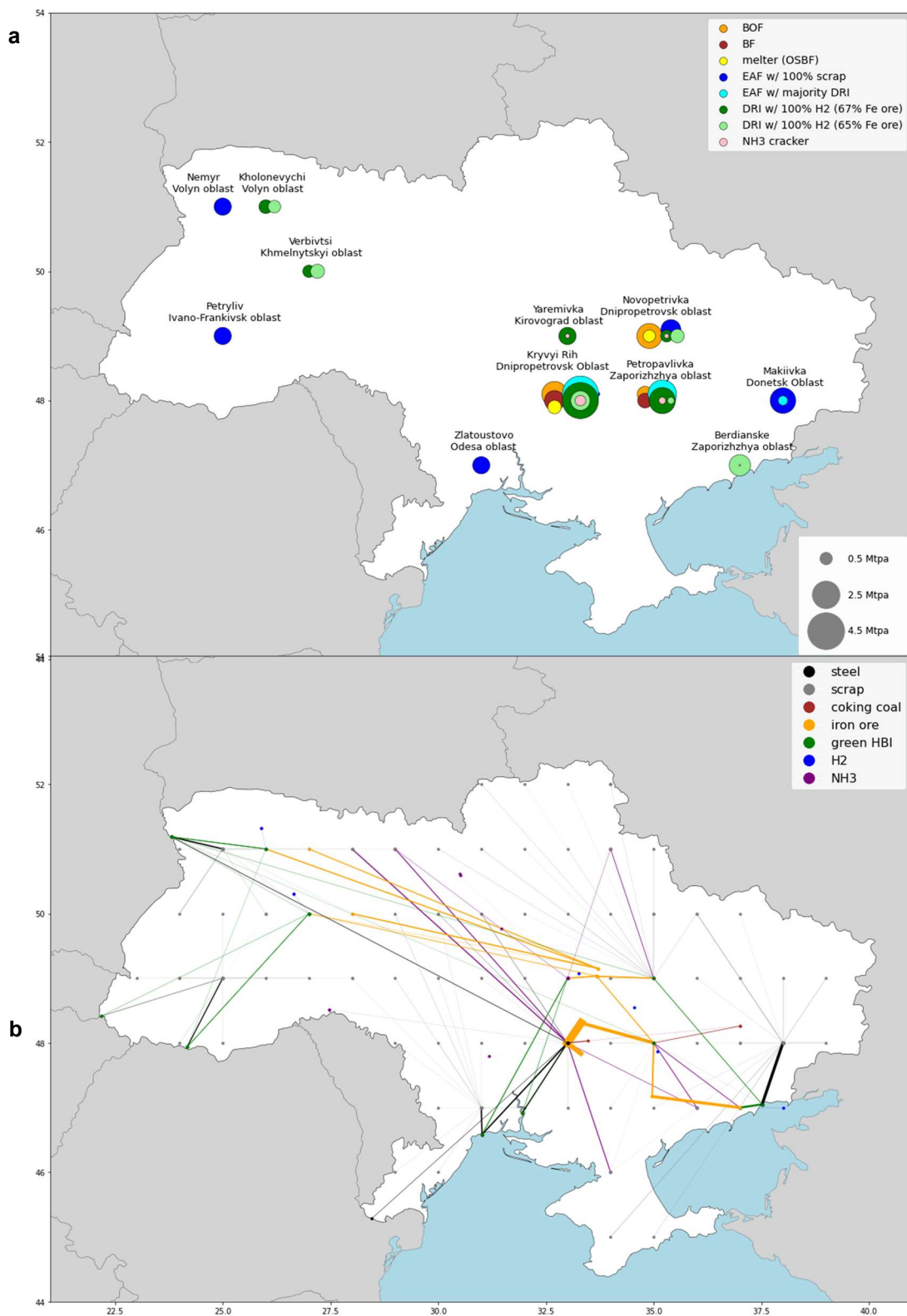


Figure S5.13 Optimised steel supply chains in 2040 under the Full Liberation & Steady Recovery Scenario: (a) capacity of iron and steel production assets (marker diameter indicates rated capacity), and (b) domestic supply chain flows (straight-line distances shown, line thickness indicates trade volume).

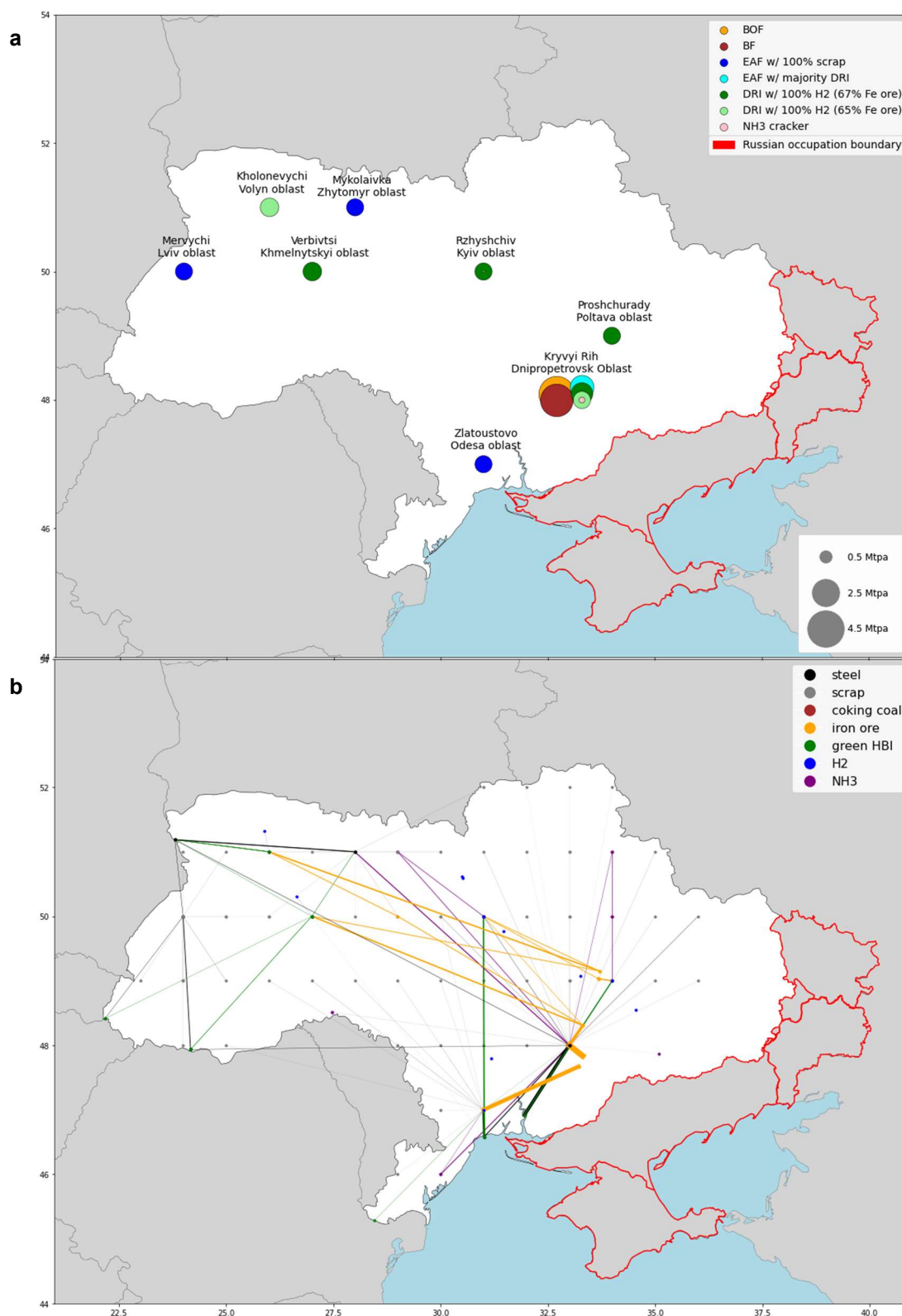


Figure S5.14 Optimised steel supply chains in 2030 under the Partial Liberation & Slow Recovery Scenario: (a) capacity of iron and steel production assets (marker diameter indicates rated capacity), and (b) domestic supply chain flows (straight-line distances shown, line thickness indicates trade volume). The geospatial data for Russian-occupied regions were provided by Deep State UA (2023), accurate as of April 2023.

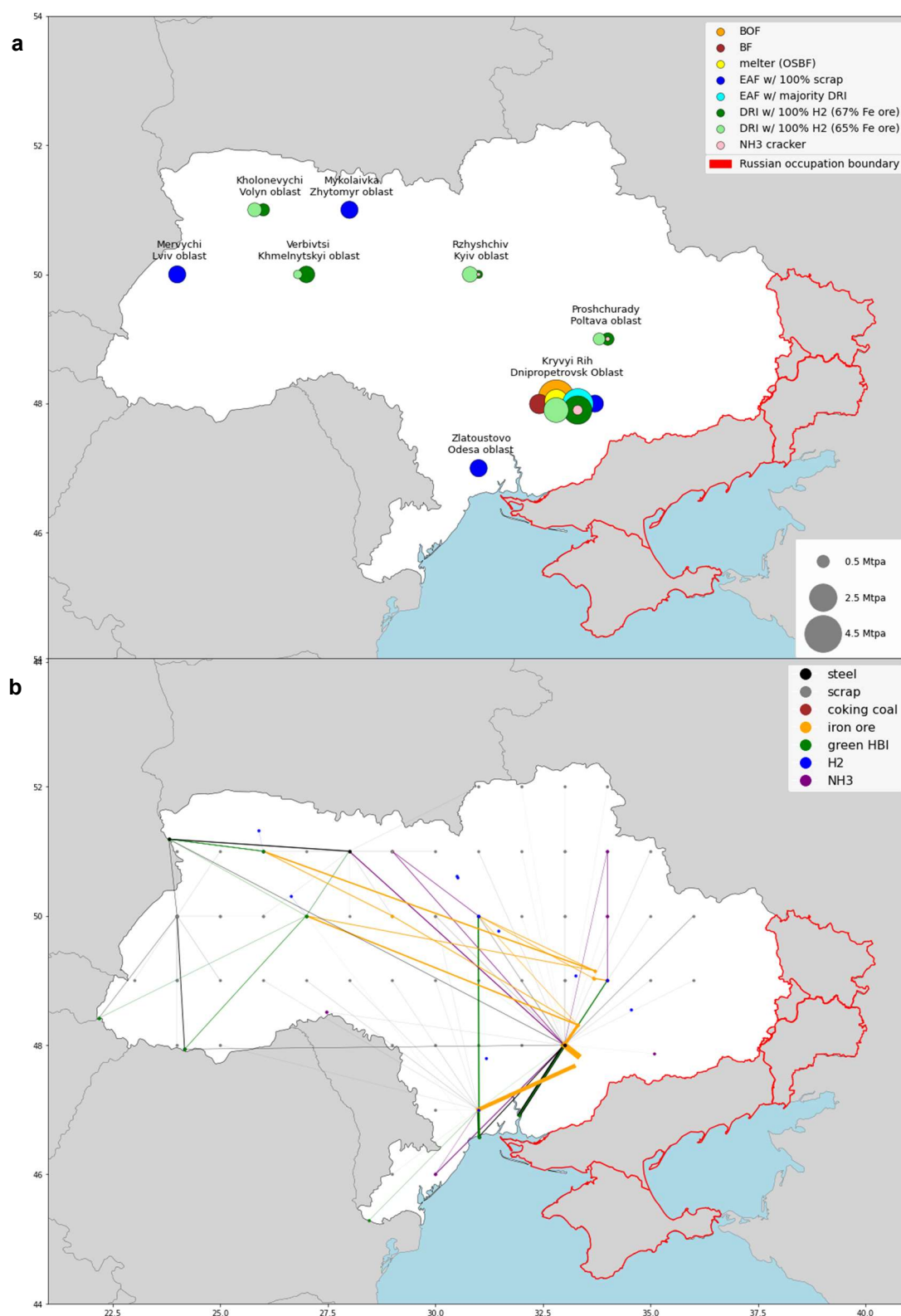


Figure S5.15 Optimised steel supply chains in 2040 under the Partial Liberation & Slow Recovery Scenario: (a) capacity of iron and steel production assets (marker diameter indicates rated capacity), and (b) domestic supply chain flows (straight-line distances shown, line thickness indicates trade volume). The geospatial data for Russian-occupied regions were provided by Deep State UA (2023), accurate as of April 2023.

Table S5.6 Energetic requirements for each optimised scenario.

		Electricity	H₂	NH₃	TOTAL	electrical +	chemical
		MWh	MWh	MWh	energy	TWh	million GJ
Full Liberation	2030	6,049,568	20,519,260	15,962,988		42.53	153
Full Liberation	2040	8,712,361	26,700,622	23,267,511		58.68	211
Full Liberation	2050	9,838,218	33,747,168	24,805,414		68.39	246
Partial Liberation	2030	2,685,120	8,118,920	4,042,818		14.85	53
Partial Liberation	2040	5,509,330	16,832,924	14,500,145		36.84	133
Partial Liberation	2050	6,091,484	21,253,312	19,728,853		47.07	169

Table S5.7 Capital requirements for energy production, by scenario.

	TOTAL		Electrolysers		Solar		Onshore wind		Offshore wind	
	MW	\$ billion	MW	\$ billion	MW	\$ billion	MW	\$ billion	MW	\$ billion
Strong Recovery Scenario		45.93		6.23		13.43		13.27		12.99
2030 New Capacity	31896	31.96	11598	4.47	8058	5.12	7450	11.55	4790	10.83
2040 Additional Capacity	15635	8.95	3781	1.29	9413	3.77	1311	1.72	1129	2.17
2050 Additional Capacity	17989	5.02	1640	0.48	16349	4.54	0	0	0	0
Slow Recovery Scenario		19.05		3.69		7.63		7.72		
2030 New Capacity	7192	5.75	2724	1.05	2437	1.55	2031	3.15	-	-
2040 Additional Capacity	16052	9.34	4570	1.55	7998	3.21	3483	4.58	-	-
2050 Additional Capacity	14074	3.97	3693	1.09	10381	2.88	0	0	-	-

Table S5.8 Capital requirements for energy storage, by scenario.

	TOTAL		Batteries		CGH ₂		NH ₃	
	-	\$ billion	MWh	\$ billion	t H ₂	\$ billion	t NH ₃	\$ billion
Strong Recovery Scenario		6.61	14840	2.84	2901	2.93	492322	0.85
2030 New Capacity	-	3.05	8242	1.71	1501	1.05	195606	0.29
2040 Additional Capacity	-	2.05	3865	0.70	218	1.05	121106	0.29
2050 Additional Capacity	-	1.52	2734	0.43	1183	0.83	175611	0.26
Slow Recovery Scenario		3.19	10076	1.85	1059	0.74	402639	0.60
2030 New Capacity	-	0.93	3228	0.67	226	0.16	68662	0.10
2040 Additional Capacity	-	1.36	4330	0.79	578	0.40	109795	0.16
2050 Additional Capacity	-	0.91	2518	0.39	254	0.18	224182	0.34

Table S5.9 Capital requirements for iron and steel production, by scenario.

	TOTAL		DRI furnaces		EAF		OSBF		NH ₃ Cracker	
	-	\$ billion	Mtpa	\$ billion	Mtpa	\$ billion	Mtpa	\$ billion	Mtpa	\$ billion
Strong Recovery Scenario		9.50	18.40	5.71	10.20	2.88	3.11	0.88	0.86	0.03
2030 New Capacity	-	5.40	10.81	3.35	7.20	2.04	0.00	0.00	0.48	0.01
2040 Additional Capacity	-	2.18	3.26	1.01	3.00	0.85	1.11	0.31	0.22	0.01
2050 Additional Capacity	-	1.91	4.33	1.34	0.00	0.00	2.00	0.57	0.16	0.00
Slow Recovery Scenario		6.34	11.20	3.47	7.17	2.03	2.92	0.83	0.59	0.01
2030 New Capacity	-	3.55	6.94	2.15	4.93	1.39	0	0	0.13	0.00
2040 Additional Capacity	-	1.81	2.14	0.66	2.25	0.63	1.77	0.50	0.30	0.00
2050 Additional Capacity	-	0.99	2.12	0.66	0.00	0.00	1.15	0.32	0.16	0.00

Economic Multipliers

Investing in the basic metals industry will cause ripple effects across the economy. In 2021, for every \$1 invested in the basic metals industry, an additional \$3.28 was generated elsewhere in the economy through indirect and induced effects (based on the Type II multiplier, see Table S5.10). In terms of domestic final demand, in addition to the basic metals industry grouping itself, the largest iron and steel consumers include fabricated metal products, and construction (for full details, see Table S5.11). The I-O multipliers of Ukraine's steel sector show a very high level of supplier linkage effects, as well as income and GVA growth effects on the broader economy.

In addition to analysing the economic impact of Ukraine's post-war construction industry's increased demand, a comparative macroeconomic assessment was undertaken of the: (i) emissions-intensive coal-based steel sector, and (ii) transitioning green steel sector associated with the *Strong Recovery* scenario. Results show that a green steel sector will benefit the economy with stronger supply chain linkages, income generation, and gross value-added under most scenarios. For the 2030 green steel sector over its 20-year project lifetime, the Ukrainian economy is forecast to generate \$446bn of steel sector-driven output, \$88bn of income, and \$269bn of GVA. The corresponding coal-based steel sector would generate less income (\$81bn) and far less GVA (\$192bn). The 2040 green steel sector appears the most impactful, generating \$1,152bn of output, \$227bn of income, and \$578bn of GVA; by contrast, the coal-based steel sector equivalent would result in a much smaller impact, with \$739bn of output, \$99bn of income, and \$235bn of GVA. The 2050 green steel scenario is characterised by a smaller impact on output (\$737bn), income (\$145bn), and GVA (\$415bn) than the 2040 scenario, but still beats the equivalent coal-based steel sector in terms of income and GVA (see Figure S5.16). I-O analysis of future green steel production is indicative as they are based on historical compositions of the electricity and chemical industries - growing renewables shares in the electricity sector and electrolytic processes for H₂ and NH₃ production will change how these sectors interact with the economy, and perhaps even bolster it. Nevertheless, a strong correlation between the proposed green steel sector and economic growth is determined.

Table S5.10 Input-output Leontief multipliers for Ukraine's basic metals and construction industries in 2014 and 2021. From authors' own calculations on the basis of Input-Output Tables from State Statistics Service of Ukraine (2022). Three types of economic impacts are assessed: direct (the immediate effect on the steel sector caused by the change in final demand), indirect (throughout the supply chain, caused by the consequent changes in intermediate demand), and induced (change in compensation of employees and other incomes, causing further spending). The output multiplier is expressed as the ratio of direct and indirect (for Type I) as well as induced (for Type II) output changes to the direct output change, based on 1-unit of currency.

	Basic Metals				Construction			
	2014		2021		2014		2021	
	Type I	Type II	Type I	Type II	Type I	Type II	Type I	Type II
Output multiplier	3.24	4.38	3.34	4.28	3.23	4.38	3.60	4.65
Income multiplier	6.68	9.45	6.67	9.24	4.07	5.77	4.65	6.44
GVA multiplier	6.56	9.75	6.38	8.80	4.26	6.32	5.15	7.37

Table S5.11 Use of domestic outputs of the '24. Basic metals' industry: aggregate combined use table (basic prices), percentage of total use, 2012-2021, and the ten-year average

Source: authors' own calculations using data from National Accounts of Ukraine, Kyiv (State Statistics Service of Ukraine, 1990-2021).

NACE	Consumers of basic metals	2012	2013	2014	2015	2016	2017	2018	2019	2020	2021	Mean
	I. Intermediate consumption by industries											
A01-A03	Agriculture, forestry & fishing	0.12	0.12	0.13	0.18	0.27	0.30	0.24	0.28	0.32	0.42	0.24
B05	Coal and lignite	0.38	0.32	0.12	0.07	0.10	0.12	0.14	0.13	0.06	0.14	0.16
B06	Crude petroleum and natural gas	0.12	0.10	0.10	0.16	0.47	0.12	0.33	0.37	0.10	0.00	0.19
B07-B09	Metal ores; other mining and quarrying; mining support services	0.69	0.58	0.85	0.52	0.75	0.94	0.91	0.80	1.15	2.15	0.93
C10-C12	Food products; beverages; tobacco products	0.45	0.27	0.24	0.29	0.51	0.64	0.61	1.53	0.40	0.37	0.53
C13-C15	Textiles; wearing apparel; leather and related products	0.00	0.01	0.00	0.02	0.04	0.05	0.01	0.01	0.01	0.02	0.02
C16-C18	Wood & of products of wood & cork, except furniture; articles of straw & plaiting materials; paper & paper products; printing and recording services	0.07	0.09	0.06	0.08	0.11	0.16	0.09	0.10	0.18	0.05	0.10
C19.1	Coke oven products	0.02	0.03	0.03	0.02	0.03	0.02	0.05	0.01	0.03	0.03	0.03
C19.2	Refined petroleum products	0.01	0.01	0.03	0.03	0.04	0.01	0.01	0.11	0.09	0.00	0.03
C20	Chemicals and chemical products	0.12	0.13	0.07	0.07	0.09	0.08	0.08	0.17	0.13	0.08	0.10
C21	Basic pharmaceutical products and pharmaceutical preparations	0.01	0.01	0.01	0.02	0.01	0.02	0.03	0.04	0.04	0.05	0.02
C22	Rubber & plastic products	0.07	0.11	0.12	0.11	0.24	0.36	0.32	0.32	0.18	0.50	0.23
C23	Other non-metallic mineral products	0.34	0.58	0.39	0.52	0.95	1.08	0.73	0.87	0.96	0.80	0.72
C24	Basic metals	12.50	8.93	9.42	10.65	14.00	15.40	14.58	10.98	11.71	12.13	12.03
C25	Fabricated metal products, except machinery and equipment	3.30	4.83	3.26	2.96	3.95	2.75	4.39	5.57	6.58	5.34	4.29
C26	Computer, electronic & optical products	0.11	0.11	0.12	0.09	0.12	0.09	0.12	0.13	0.12	0.07	0.11
C27	Electrical equipment	0.39	1.75	1.21	0.87	0.96	0.86	0.91	1.41	1.08	0.95	1.04
C28	Machinery and equipment n.e.c.	2.49	2.76	1.76	1.66	1.45	1.67	1.28	2.05	1.66	1.73	1.85
C29	Motor vehicles, trailers and semi-trailers	0.58	0.37	0.12	0.01	0.13	0.20	0.19	0.40	0.00	0.17	0.22
C30	Other transport equipment	4.91	3.15	1.21	0.47	0.58	0.66	0.81	1.34	1.18	0.66	1.50
C31-C33	Furniture; other manufactured goods; repair & installation of machinery and equipment	1.05	0.73	0.59	0.68	0.70	1.26	0.89	1.56	1.39	1.72	1.06
D35	Electricity, gas, steam and air conditioning supply	2.24	2.69	3.04	2.86	2.93	3.82	3.10	3.89	5.61	3.58	3.38

E36-E39	Water supply; sewerage; waste management and remediation	0.63	0.93	1.92	1.08	1.48	1.34	1.11	1.42	1.15	0.74	1.18
F41-F43	Construction	4.85	4.94	3.89	2.72	2.59	2.93	3.33	4.93	5.30	3.83	3.93
G45-G47	Wholesale and retail trade; repair of motor vehicles and motorcycles	0.23	0.39	0.51	0.30	0.86	1.17	1.00	1.20	1.06	1.38	0.81
H49-H52	Land transport; water transport; air transport; warehousing & transport support	0.22	0.15	0.32	0.19	0.16	0.14	0.11	0.27	0.44	0.19	0.22
H53	Postal & courier services	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
I55-I56	Accommodation; food & beverage services	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.01	0.00	0.01	0.01
J58-J60	Publishing; motion picture, video & TV programme production; sound recording, programming and broadcasting services	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
J61	Telecommunications	0.01	0.01	0.01	0.01	0.01	0.00	0.00	0.01	0.00	0.00	0.01
J62-J63	Computer programming & consultancy services; information services	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.01	0.00	0.00
K64-K66	Financial services; insurance, reinsurance and pension funding, excl. compulsory social security; activities auxiliary to financial services	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
L68	Real estate activities	0.08	0.06	0.15	0.05	0.00	0.10	0.10	0.19	0.20	0.21	0.11
M69-M71	Legal and accounting services; activities of head offices; management consultancy activities; architectural & engineering services; technical testing & analysis	0.09	0.07	0.07	0.10	0.22	0.19	0.24	0.11	0.14	0.11	0.13
M72	Scientific research & development	0.08	0.11	0.05	0.04	0.04	0.04	0.03	0.05	0.09	0.04	0.06
M73-M75	Advertising & market research; other professional, scientific and technical services; veterinary services	0.01	0.02	0.01	0.00	0.06	0.05	0.04	0.14	0.17	0.19	0.07
N77-N82	Administrative and support service activities	0.02	0.03	0.02	0.02	0.03	0.05	0.02	0.06	0.06	0.05	0.04
O84	Public administration and defence; compulsory social security	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
P85	Education	0.00	0.00	0.01	0.01	0.00	0.01	0.01	0.01	0.01	0.00	0.01
Q86-Q88	Human health and Social Work activities	0.00	0.00	0.00	0.01	0.00	0.01	0.01	0.00	0.01	0.00	0.00
R90-R93	Arts, Entertainment and recreation	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
S94-S96, T97	Other service activities; activities of households	0.00	0.01	0.01	0.01	0.02	0.01	0.02	0.01	0.01	0.01	0.01
	Total intermediate demand	36.09	34.39	29.87	26.86	33.94	36.67	35.86	40.51	41.62	37.75	35.36
	II. Final consumption expenditure											
P.3	Total	0.05	0.01	0.04	0.06	0.06	0.05	0.05	0.06	0.05	0.04	0.05
P.31; S.14	Households	0.05	0.01	0.04	0.06	0.05	0.04	0.05	0.06	0.05	0.04	0.05
P.31; S.15	Non-profit institutions serving households	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
P.31, P.32; S.13	General government	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	III. Gross capital formation											

P.5g	Total	-0.34	-1.10	-1.30	0.28	2.85	0.08	0.52	0.36	-2.66	-1.64	-0.30
P.51g	Gross fixed capital formation	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
P.52	Changes in inventories	-0.34	-1.10	-1.30	0.28	2.85	0.08	0.52	0.36	-2.66	-1.64	-0.30
P.53	Net acquisitions of valuables	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	IV. Exports											
P.6	Exports of goods and services	64.20	66.70	71.38	72.80	63.15	63.21	63.57	59.06	60.99	63.85	64.89
	Total use of domestic production at basic prices	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00

Table S5.12 Applying the multiplier - economic impact of the additional \$12.63bn of post-war reconstruction demand, US\$ in current prices, average per year

NACE Code	Industry group	Initial effect	Type I multipliers	Type II multipliers	Type I multipliers	Type II multipliers	Type I multipliers	Type II multipliers
			Output		Income		GVA	
A01-A03	Agriculture, forestry & fishing	0.00	0.11	1.38	0.01	0.14	0.05	0.58
B05	Coal and lignite	0.00	0.75	0.97	0.16	0.20	0.33	0.42
B06	Crude petroleum and natural gas	0.00	1.21	1.78	0.11	0.16	0.88	1.29
B07-B09	Metal ores; other mining and quarrying; mining support services	0.00	1.73	1.86	0.19	0.21	0.76	0.82
C10-C12	Food products; beverages; tobacco products	0.00	0.01	1.33	0.00	0.13	0.00	0.26
C13-C15	Textiles; wearing apparel; leather and related products	0.00	0.03	0.27	0.01	0.07	0.01	0.13
C16-C18	Wood & of products of wood & cork, except furniture; articles of straw & plaiting materials; paper & paper products; printing and recording services	0.00	0.31	0.50	0.03	0.05	0.07	0.11
C19.1	Coke oven products	0.00	0.42	0.48	0.02	0.02	0.04	0.05
C19.2	Refined petroleum products	0.00	0.82	1.11	0.05	0.07	0.11	0.15
C20	Chemicals and chemical products	0.00	0.84	1.32	0.08	0.12	0.09	0.15
C21	Basic pharmaceutical products and pharmaceutical preparations	0.00	0.03	0.26	0.00	0.05	0.01	0.08
C22	Rubber & plastic products	0.00	0.90	1.11	0.08	0.10	0.12	0.15
C23	Other non-metallic mineral products	0.00	3.13	3.31	0.29	0.31	0.50	0.53
C24	Basic metals	0.00	2.45	2.77	0.15	0.17	0.38	0.43
C25	Fabricated metal products, except machinery and equipment	0.00	1.28	1.43	0.18	0.20	0.25	0.28
C26	Computer, electronic & optical products	0.00	0.21	0.35	0.05	0.08	0.05	0.09

<i>C27</i>	Electrical equipment	0.00	0.40	0.48	0.08	0.09	0.11	0.13
<i>C28</i>	Machinery and equipment n.e.c.	0.00	0.53	0.69	0.13	0.17	0.16	0.21
<i>C29</i>	Motor vehicles, trailers and semi-trailers	0.00	0.34	0.63	0.11	0.20	0.07	0.14
<i>C30</i>	Other transport equipment	0.00	0.08	0.11	0.02	0.03	0.03	0.04
<i>C31-C33</i>	Furniture; other manufactured goods; repair & installation of machinery and equipment	0.00	0.22	0.39	0.05	0.09	0.08	0.14
<i>D35</i>	Electricity, gas, steam and air conditioning supply	0.00	1.82	2.62	0.26	0.38	0.54	0.78
<i>E36-E39</i>	Water supply; sewerage; waste management and remediation	0.00	0.10	0.17	0.03	0.05	0.03	0.05
<i>F41-F43</i>	Construction	12.63	20.55	20.87	2.04	2.07	3.85	3.91
<i>G45-G47</i>	Wholesale and retail trade; repair of motor vehicles and motorcycles	0.00	3.41	5.62	0.71	1.17	1.67	2.76
<i>H49-H52</i>	Land transport; water transport; air transport; warehousing & transport support	0.00	1.52	2.20	0.40	0.58	0.66	0.96
<i>H53</i>	Postal & courier services	0.00	0.01	0.03	0.01	0.01	0.01	0.02
<i>I55-I56</i>	Accommodation; food & beverage services	0.00	0.03	0.22	0.00	0.03	0.02	0.12
<i>J58-J60</i>	Publishing; motion picture, video & TV programme production; sound recording, programming and broadcasting services	0.00	0.11	0.18	0.02	0.04	0.04	0.07
<i>J61</i>	Telecommunications	0.00	0.04	0.18	0.01	0.04	0.02	0.10
<i>J62-J63</i>	Computer programming & consultancy services; information services	0.00	0.16	0.27	0.02	0.04	0.09	0.15
<i>K64-K66</i>	Financial services; insurance, reinsurance and pension funding, excl. compulsory social security; activities auxiliary to financial services	0.00	0.53	0.88	0.15	0.25	0.35	0.58
<i>L68</i>	Real estate activities	0.00	0.26	0.92	0.02	0.09	0.19	0.68
<i>M69-M71</i>	Legal and accounting services; activities of head offices; management consultancy activities; architectural & engineering services; technical testing & analysis	0.00	0.45	0.63	0.11	0.15	0.20	0.28
<i>M72</i>	Scientific research & development	0.00	0.02	0.03	0.01	0.01	0.01	0.02
<i>M73-M75</i>	Advertising & market research; other professional, scientific and technical services; veterinary services	0.00	0.18	0.35	0.03	0.06	0.10	0.19
<i>N77-N82</i>	Administrative service activities and support	0.00	0.31	0.50	0.10	0.17	0.16	0.26
<i>O84</i>	Public administration and defence; compulsory social security	0.00	0.12	0.17	0.08	0.12	0.09	0.13
<i>P85</i>	Education	0.00	0.01	0.09	0.01	0.06	0.01	0.06
<i>Q86-Q88</i>	Human health and Social Work activities	0.00	0.01	0.11	0.00	0.05	0.00	0.05
<i>R90-R93</i>	Arts, Entertainment and recreation	0.00	0.01	0.05	0.00	0.02	0.00	0.03
<i>S94-S96, T97</i>	Other service activities; activities of households	0.00	0.01	0.08	0.00	0.02	0.01	0.05
	Total	12.63	45.46	58.70	5.83	8.08	12.18	17.44

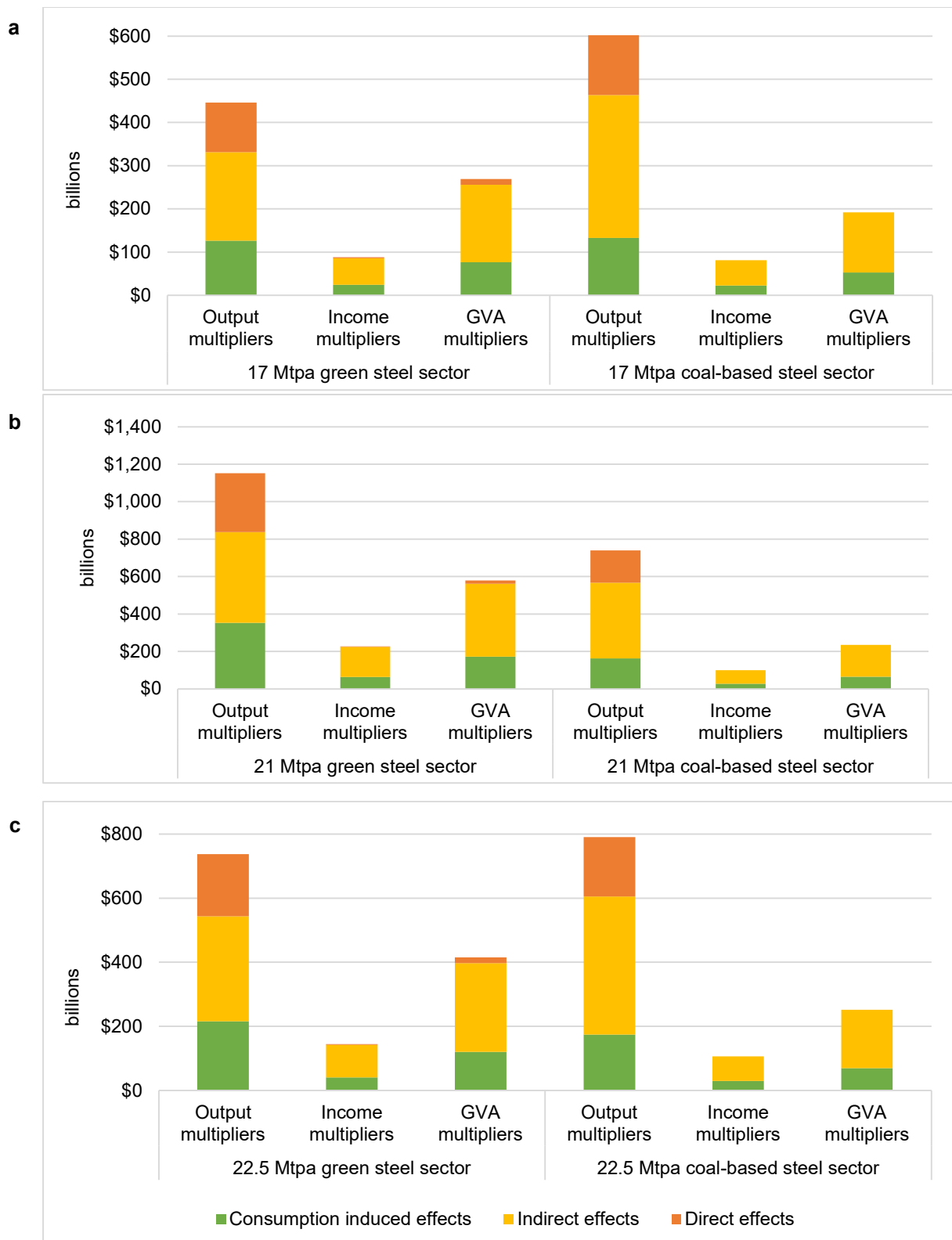


Figure S5.16 The macroeconomic effects of steel production, quantified in terms of output, income and GVA multipliers over a 20-year project lifetime, and compared across two distinct sectorial pathways: (i) the green steel sector (based on the Strong Recovery scenario), and (ii) the coal-based steel sector (based on pre-war 2021 economic multipliers). Demonstrated for (a) steel output of 17.2 Mtpa, equivalent to the 2030 Strong Recovery scenario, (b) steel output of 21.1 Mtpa, equivalent to the 2040 Strong Recovery scenario, and (c) steel output of 22.5 Mtpa, equivalent to the 2050 Strong Recovery scenario.

A.iii.2 Supplementary Methods

Near zero-carbon electricity, hydrogen, and ammonia production

The challenge of using renewable energy to produce green hydrogen and ammonia is the variability of the renewable energy resource. If downstream equipment, like the electrolyser (which is the biggest consumer of energy), is equal in size to the renewable energy plant, then it will sit idle whenever renewable energy is not available. On the flipside, if the electrolyser is much smaller than the renewable energy plant, then energy will be curtailed whenever the plant generates at its maximum rate. Optimisation tools are needed to strike a balance between these requirements to prevent wastage of electricity or low utilisation of downstream equipment. These tools also enable other considerations to be included, including (i) whether only wind, only solar, or a hybrid of both, achieves the lowest costs; (ii) whether production of chemical fuels should be smoothed out using buffer storage downstream (which in the case of hydrogen is very expensive), or by oversizing of renewables upstream (which will increase curtailment); (iii) the constraints introduced by equipment with limited flexibility, like the Haber-Bosch plant, which cannot be turned off entirely and must always operate at or above a minimum fraction of its design rate (a number of values are used for this minimum design rate in the literature – a conservative value of 30% is adopted here).

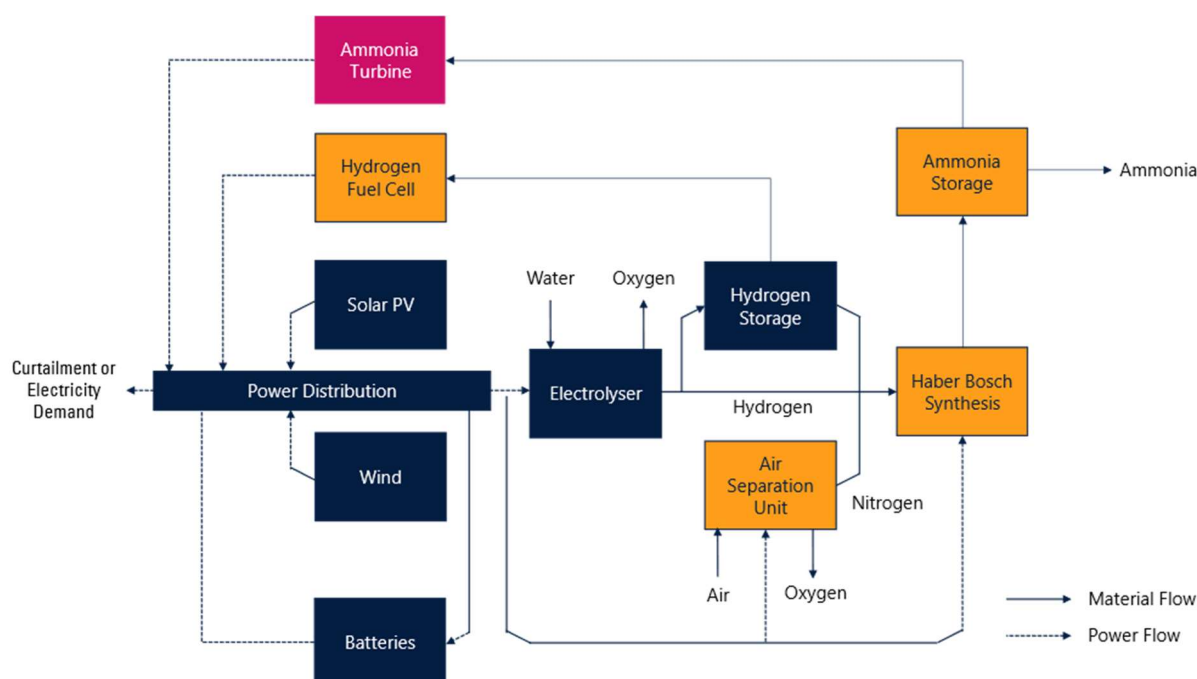


Figure S5.17 System for the production of hydrogen, ammonia, and electricity. The size of each unit is determined by an optimisation model, which minimises the net present value of the system, using the capital cost of each unit, and weather data, which determines the output of electricity in each hour from the installed wind and solar plants. In the hydrogen case, a constant load of hydrogen must be produced using only the units in dark blue (Solar PV, wind, power distribution, electrolysis, hydrogen storage and batteries); for the ammonia case, a constant ammonia stream must be produced, using the same units as for hydrogen and the units in orange (Air separation unit, Haber-Bosch synthesis, a hydrogen fuel cell and ammonia storage); for the electricity case, a near constant electricity demand must be met – any unit can be used.

The land area available to install RE infrastructure (solar PV panels and onshore wind turbines) for green steel production was assessed for all 73 land-based grids. Factors were applied to determine the land available for renewables which depended on the land type classification ($f_{RE_{land_class}}$). Land classifications were defined by the MODIS5 dataset (Friedl & Sulla-Menashe, 2019) and RE reduction factors are shown in Table S5.13. An additional reduction factor of 0.2 was applied to account for the portion of total RE land availability that the steel sector may consume (f_{steel}), which matches the pre-war energy consumption of the steel sector as portion of Ukrainian final energy consumption.

$$Land_Available_SteelRE^{grid} = \sum_{land_class} T_{land}^{grid}_{land_class} * f_{RE_{land_class}} * f_{steel} \quad \forall grid$$

The sea area available to install RE infrastructure (offshore wind turbines) for green steel production was similarly assessed, however, a single RE reduction factor was applied for all locations.

$$Sea_Available_SteelRE^{grid} = T_{sea}^{grid} * f_{RE_{sea}} * f_{steel} \quad \forall grid$$

Table S5.13 Fraction of land available for renewables according to land classification (Salmon & Bañares-Alcántara, 2022)

Land Cover Type	MODIS Number	Fraction of land available for renewables	
		Wind	Solar
Evergreen Needleleaf Forests	1	-	-
Evergreen Broadleaf Forests	2	-	-
Deciduous Needleleaf Forests	3	-	-
Deciduous Broadleaf Forests	4	-	-
Mixed Forests	5	-	-
Closed Shrublands	6	0.5	0.5
Open Shrublands	7	0.5	0.5
Woody Savannas	8	0.2	0.2
Savannas	9	0.2	0.2
Grasslands	10	0.2	0.2
Permanent Wetlands	11	-	-
Croplands	12	0.1	0.05
Urban and Built-up Lands	13	-	0.03
Cropland, Natural Vegetation, Mosaic	14	0.1	0.05
Permanent Snow and Ice	15	-	-
Barren	16	1	1
Water Bodies	17	-	-

Table S5.14 Solar and wind power plants commissioned in Ukraine, used as basis for learning curve projections to 2050.

Name	Location	Investments	MW	Commissioning date	1MW costs (USD/MW)
Nikopol SPP	Dnipropetrovsk region	€230m	246MW	Mar-19	1028455
Pokrovskaya SPP	Dnipropetrovsk region	€200m	240MW	Oct-19	916666
Kamianets-Podilskyi SPP	Khmelnyskyi	\$55m	64MW	Mar-19	945313
Yavoriv Solar	Lviv region (West)	€34.7m	36MW	Oct-18	1069444
Tokmak SPP	Zaporizhzhia Oblast	€45m	50MW	Apr-18	990000
Botievskaya WPP	Zaporizhzhia Oblast	€340m	200MW	2014	1870000
Primorskaya WPP	Zaporizhzhia Oblast	€321m	200MW	2019	1765500
Orlovksa WPP	Zaporizhzhia Oblast	€131m	100MW	2019	1441000
Myrnska WPP	Kherson oblast	€326m	164MW	2019	2186584
Overyanivska WPP	Kherson oblast	€118m	70MW	2019	1854285

Table S5.15. Time-variable cost parameters for renewable energy and hydrogen production and storage

	UA/global data	Unit	2022	2030	2040	2050	Source/notes
Onshore wind turbine	UA	mil \$/MW	1.823	1.550	1.314	1.151	2022 value from actual installed projects in Ukraine, then learning curves applied
Offshore fixed bottom wind turbine	global	mil \$/MW	2.660	2.260	1.920	1.680	Salmon and Bañares-Alcántara (2022)
Offshore floating bottom wind turbine	global	mil \$/MW	2.990	2.540	2.150	1.890	Salmon and Bañares-Alcántara (2022)
Land-based solar panel	UA	mil \$/MW	0.990	0.635	0.401	0.277	2022 value from actual installed projects in Ukraine, then learning curves applied
Electrolysers (low-temperature)	global	mil \$/MW	-	0.385	0.340	0.295	IEA (2021b)
Lithium-ion batteries	global	mil \$/MWh	-	0.207	0.182	0.156	Cole and Frazier (2020)
Hydrogen fuel cell	global	mil \$/MW	-	0.457	0.267	0.218	Whiston et al. (2019)
CGH ₂ storage vessel (200 bar)	global	mil \$/MW	-	0.70	0.70	0.70	Abdin et al. (2021)

Table S5.16. Time-variable efficiency of electrolysis and fuel cells

	UA/global data	Unit	2022	2030	2040	2050	Source/notes
Electrolyser efficiency	global	% (LHV)	-	68%	72%	75%	IEA (2019)
FC efficiency	global	% (LHV)	-	60%	62%	64%	IEA (2015)

Table S5.17. Energy and cost parameters for ammonia production

	UA/global data	Unit	Value	Source/notes
Haber Bosch Electricity Consumption	global	MWh/t NH ₃	1	IRENA (2022a)
Haber Bosch Plant	global	USD/tpa NH ₃ (rated capacity)	700	
Liquefied NH ₃ storage vessel	global	USD/t NH ₃ (peak capacity)	1500	

Dynamic material flow analysis

To determine post-consumer steel outflows, the lifetime probability distribution function was applied to inflows, according to the steel product category (assuming continuous distribution):

$$Outflow(t, c) = \frac{stock(t'_0)}{(t - t'_0)} + \sum_{t' < t} Inflow(t', c) * f(t, t', \tau(c), \sigma(c)) \quad (Eqn S5.1)$$

$$f(t, t', \tau(c), \sigma(c)) = \frac{1}{\sigma\sqrt{2\pi}} * \exp\left(\frac{-(t - t' - \tau)^2}{2\sigma^2}\right) \quad (Eqn S5.2)$$

Where $f(t, t', \tau, \sigma)$ is the lifetime probability distribution function, t is the model year (2030, 2040, 2050), t' is the cohort of steel product (1900-2070), τ is the lifetime of the product category and σ is the standard deviation of the lifetime, as defined in the table below.

Table S5.18 Ukrainian in-use steel stocks in 1900, lifetime and standard deviation by steel product category, based on per capita stock estimates from S Pauliuk et al. (2013) for the former-USSR region.

	<i>Ukraine in use stocks, 1900</i>	<i>Lifetime</i>	<i>Standard deviation of the lifetime</i>
Product category (c)	(kt)	τ (years)	σ (years)
<i>Transportation</i>	1872	20	6.00
<i>Machinery</i>	839	30	9.00
<i>Construction</i>	5279	75	22.50
<i>Appliances/packaging</i>	740	15	4.50

Iron and steel production and trade

Establishing the model

Energy can be drawn from fossil fuels (metallurgical coal, natural gas), renewables (hybrid onshore solar and wind, offshore wind, hydropower), or near-zero carbon alternatives (nuclear power). Newly installed solar and wind plants and existing hydro and nuclear power plants could produce electricity, hydrogen, and/or ammonia for use in steel production. Electricity could be transmitted and distributed via the network, hydrogen transported in compressed gaseous form within freight trucks or pipelines, and ammonia transported in liquid form within pipelines.

Process flexibility and energy storage are critical in managing renewable energy sources (RES) for cost-effective industrial operations. Whilst oversizing of renewable energy production infrastructure (i.e., solar panels and wind turbines) is essential since the wind does not always blow nor the sun always shine, it becomes an operational choice to make hydrogen and/or steel production flexible (thereby oversizing electrolyser and furnace capacities, respectively, and providing relevant energy/material storage facilities). The broad requirement for continuous DRI operations to ensure a uniform oxidation front was shown in previous work (Devlin et al., 2023) to limit the benefits of EAF flexibility. Hence, at the facility-level, this study focuses on optimising upstream electricity and hydrogen production.

The following supply chain network features framed the model:

- (1) Within a country, commodities can be moved between (production) sites and ports;
- (2) Internationally, commodities can be moved between ports or rail border crossings;
- (3) Raw materials into iron and steelmaking (called "RawMat") must be supplied locally at a site or transported from suppliers in the case of electricity, H₂, NH₃, metallurgical coal, iron ore and natural gas;
- (4) On each site, any production activities can happen and any raw materials can be supplied;
- (5) A production activity will consume feeds;
- (6) H₂ can be supplied as a primary resource or as a product from NH₃ cracking (which is a production activity);
- (7) Any site or port can provide a product to directly contribute to meeting the national demand; transporting products to a demand centre in a country is not modelled (steel demand can be met at any grid/port as we don't know where finishing processes will occur);
- (8) Commodities produced by offshore, HPP or NPP can only be moved from their origin to a site, not between sites; they can effectively be exchanged between sites, not directly but after they have become part of RawMatSupply at a site for elec, H₂ or NH₃.

Steel production routes

In addition to the conventional integrated BF-BOF and scrap-based EAF routes, the following possible low- and near-zero emissions ironmaking routes were modelled:

- DRI with 100% H₂ feedstock (67%-Fe or 65%-Fe ore)
- DRI with 65% H₂ feedstock (minimum amount of NG to maintain DRI of 3.5%-carbon(C); 67%-Fe ore)
- DRI with 70% NG feedstock (maximum amount of H₂ without altering NG-DRI infrastructure; 67%-Fe ore)
- DRI with 100% NG feedstock (67%-Fe or 65%-Fe ore)

Iron was fed into the following possible steelmaking routes (OHF excluded as outdated, inefficient technology):

- EAF charged with 86% DRI (of 0%-C or 3.5%-C, produced using 67%-Fe ore), 14% scrap
- BOF charged with 89% DRI (of 0%-C or 3.5%-C, produced using 65%-Fe ore), 11% scrap, combined with pre-BOF melter unit (OSBF)

Hence, there are eight possible iron and steelmaking routes considered, with semi-finished steel as the final product:

- BF-BOF
- scrap-EAF
- 100% H₂-DRI-EAF
- 100% NG-DRI-EAF
- 70% NG-DRI-EAF
- 65% H₂-DRI-EAF
- 100% NG-DRI-OSBF-BOF
- 100% H₂-DRI-OSBF-BOF

Insufficient iron quality is a major concern for upscaling production using DR shaft furnaces. Due to the production of sponge iron in DRI operations (rather than molten iron as in BF operations with slag production), ore gangue is preserved. Hence, ore of higher quality must be fed into the furnace, of around 67%-Fe content (Barrington, 2018). The average global in-situ Fe-content of iron ore deposits is 47%, and for Ukraine, this is 35%, both far less than the extracted ore Fe-content due to the preferential extraction of higher quality ores (U.S. Geological Survey, 2022). Significant beneficiation will be required to deliver direct reduction (DR)-grade ore. Alternatively, BF-grade ore can be used so long as DRI is followed by an extra electric smelting unit (similar to the EAF) before BOF steelmaking, to melt the sponge iron into molten iron and remove impurities. This process is advantageous in using existing assets and lower quality ore (Cavaliere et al., 2022; Zulli, 2022). Therefore, this study investigates both the DRI-EAF route, which demands higher-quality 67%-Fe ore, and the DRI-melter-BOF route, which requires 65%-Fe ore.

The continuation of any OHF assets is not considered for any scenario as it is outdated, inefficient technology. In 2008, the BF-OHF route represented 2.2% of global production, but 41.3% of Ukraine's production (worldsteel, 2010). Within the next decade to 2018, BF-OHF production dropped to 0.4% of global production yet persisted in Ukraine with 22.9% of production; Russia is the only other country where OHFs still exist (worldsteel, 2020a). OHF is outdated technology of the early 1900s (Basil Turner, 1900); in comparison to the BF-OHF route, the BF-BOF route consumes 25% less energy (Morfeldt et al., 2015) and emits 8% less CO₂ due to the reduction in the use of fossil fuel firing (e.g., natural gas, fuel oil, coal or tar) across the surface of the steel bath for heating and carbon reduction (IPCC, 2019).

Key sets

Key sets were processes, products (output of processes), commodities (which can be transported), and locations.

Table S5.19 Commodity sets and subsets

Set Declaration	Elements
Commodity	ore67pel (67%-Fe ore pellets), ore65pel, ore65lump, ore65fines, ore65sinter, HBI-C0-67o (HBI with 0%-C content and produced using 67%-Fe ore), HBI-C4-67o, HBI-C0-65o, HBI-C4-65o, pigi (pig iron), SFS (semi-finished steel), elec (electricity), RE (onshore renewable energy), offRE (offshore renewable energy), HP (hydropower), NP (nuclear power), H ₂ (hydrogen), greenH ₂ (electrolytic H ₂ produced using onshore hybrid solar/wind), offgreenH ₂ (electrolytic H ₂ produced using offshore wind), pinkH ₂ (electrolytic H ₂ produced using nuclear power), hydroH ₂ (electrolytic H ₂ produced using hydropower), NH ₃ , greenNH ₃ , offgreenNH ₃ , pinkNH ₃ , hydroNH ₃ , NG (natural gas), coke, metcoal (metallurgical coal), scrap, lime, limestone, alloys, oxygen, carbon, electrode, refractory, labour
DemandCom(Commodity)	SFS, HBI-C0-67o, HBI-C0-65o
Electricity(Commodity)	RE, offRE, NP, HP
Hydrogen(Commodity)	greenH ₂ , offgreenH ₂ , pinkH ₂ , hydroH ₂
Ammonia(Commodity)	greenNH ₃ , offgreenNH ₃ , pinkNH ₃ , hydroNH ₃
SpecialCommodity (Commodity)	RE, offRE, NP, HP, greenH ₂ , offgreenH ₂ , pinkH ₂ , hydroH ₂ , greenNH ₃ , offgreenNH ₃ , pinkNH ₃ , hydroNH ₃
Product(Commodity)	ore65sinter, coke, HBI-C0-67o, HBI-C4-67o, HBI-C0-65o, HBI-C4-65o, pigi, SFS, H ₂
Feed(Commodity)	ore67pel, ore65pel, ore65lump, ore65fines, ore65sinter, elec, H ₂ , NH ₃ , NG, metcoal, coke, scrap, HBI-C0-67o, HBI-C4-67o, HBI-C0-65o, HBI-C4-65o, pigi, lime, limestone, alloys, oxygen, carbon, electrode, refractory, labor
RawMat(Commodity)	elec, H ₂ , NH ₃ , scrap, lime, limestone, alloys, oxygen, carbon, electrode, refractory, labour
TransportableCommodity* (Commodity)	elec, H ₂ , NH ₃ , ore67pel, ore65pel, ore65lump, ore65fines, HBI-C0-67o, HBI-C4-67o, HBI-C0-65o, HBI-C4-65o, SFS, RE, offRE, HP, NP, greenH ₂ , offgreenH ₂ , pinkH ₂ , hydroH ₂ , greenNH ₃ , offgreenNH ₃ , pinkNH ₃ , hydroNH ₃ , NG, metcoal, scrap
bulk(Commodity)	ore67pel, ore65pel, ore65lump, ore65fines, HBI-C0-67o, HBI-C4-67o, HBI-C0-65o, HBI-C4-65o, SFS, metcoal, scrap

*transport of lime, limestone, alloys, oxygen, carbon, electrodes, and refractories are ignored because there are no constraints on availability

Table S5.20 Process-related sets and subsets

Set Declaration	Elements
Process	sintering, coking, BF, BOF, DRIwH ₂ -67o, DRIwNG-67o, DRIw65H ₂ -67o, DRIw70NG-67o, DRIwH ₂ -65o, DRIwNG-65o, OSBFwDRI-C0, OSBFwDRI-C4, EAFwDRI-C0, EAFwDRI-C4, EAFwscrap, cracking
ExFurnace	exDRP, exEAF, exBF, exBOF
Brownfield (ExFurnace,Process)	exDRP.(DRIwH ₂ -65o, DRIwH ₂ -67o, DRIwNG-65o, DRIwNG-67o, DRIw70NG-67o, DRIw65H ₂ -67o), exEAF.(EAFwDRI-C0, EAFwDRI-C4, EAFwscrap), exBF.BF, exBOF.BOF

Table S5.21 Location sets and subsets

Set Declaration	Definition	Elements
Location	All locations	s01*s73, ow01*ow14, p01*p18, r01*r12, o01*o11, m01*m07, n01*n07, NPP1*NPP2, HPP1*HPP9
Site(Location)	Manufacturing sites	s01*s73
OffshoreSite(Location)	Offshore wind energy production sites	ow01*ow14
Port(Location)	Sea port capable of handling dry bulk commodities	p01*p18
RailX(Location)	railway crossings capable of handling dry bulk commodities	r01*r12
OreMine(Location)	iron ore mines	o01*o11
CoalMine(Location)	metallurgical coal mines	m01*m07
GasField(Location)	natural gas field or processing plant	n01*n07
NPP(Location)	nuclear power plant	NPP1*NPP2
HPP(Location)	hydro power plant	HPP1*HPP9

Table S5.22 Sets to group country with supply chain elements

Set Declaration	Elements
Country	UA (Ukraine), IT (Italy), ES (Spain), PO (Poland), RO (Romania), BG (Bulgaria), UK (United Kingdom), DE (Germany), FR (France), BE (Belgium), NL (Netherlands), PT (Portugal), CZ (Czech Republic), AT (Austria), HU (Hungary)
CountrySite(Country, Site)	UA.(s01*s73)
CountryOffshoreSite(Country, OffshoreSite)	UA.(ow01*ow14)
CountryPort(Country, Port)	UA.(p01*p05), IT.(p06*p07), ES.(p08*p09), UK.p10, DE.(p11*p12), FR.(p13*p14), BE.p15, NL.p16, PT.p17, PO.p18
CountryRailX (Country, RailX) <i>railX must be associated with both countries either side of crossing</i>	PO.r01, RO.(r02*r03), BG.(r04*r05), DE.r06, FR.r07, BE.r08, CZ.r09, NL.r10, AT.r11, HU.r12/
CountryOreMine(Country, OreMine)	UA.(o01*o11)
CountryCoalMine(Country, CoalMine)	UA.(m01*m07)
CountryGasField(Country, GasField)	UA.(n01*n07)
CountryNPP(Country, NPP)	UA.NPP1*NPP2
CountryHPP(Country, HPP)	UA.(HPP1*HPP2)

Overall mass and energy balances

(i) **Process Balance** - Feed consumption (FC) is equal to specific consumption (SC) of the feed in each process, multiplied by the manufactured product output (ProdOut):

$$FC^{site, feed} = \sum_{process} SC_{process}^{feed} * ProdOut_{process}^{site} \quad \forall \text{ site, feed} \quad (Eqn S5.3)$$

Specific consumption rates collected from a range of sources, most of which were used in a previous study (Devlin et al., 2023) with additional data from Müller et al. (2021) and Jacobasch et al. (2021) for H₂/NG blends in DRI, Cavaliere et al. (2022) for the DRI-OSBF-EAF route, and IEAGHG (2013) for the conventional BF-BOF, among others. Specific consumption rates are detailed in Table S.2.12.

(ii) Site Balance – The site's incoming commodities, accounted for as local raw material supply (RawMatSup), manufactured product output and/or received freight by national transportation (NatTrans), must equal the site's outgoing commodities, accounted for as feed consumption, national demand contributions (NatDemCont) and/or dispatched freight by national transportation.

$$\begin{aligned} RawMatSup_{cmdty}^{site} + \sum_{process} ProdOut_{process}^{site} + \sum_{location'} NatTrans_{cmdty}^{location',site} \\ = FC_{cmdty}^{site} + NatDemCont_{cmdty}^{site} + \sum_{location'} NatTrans_{cmdty}^{site,location'} \end{aligned} \quad (Eqn S5.4)$$

Repeated for all sites and transportable commodities.

$$\forall site, cmdty$$

(iii) Port Balance - The port's incoming commodities, which includes received freight by national or international (imports) transportation, must equal the site's outgoing commodities, accounted for as national demand contributions and/or dispatched freight by national or international (exports) transportation.

$$\begin{aligned} \sum_{site'} NatTrans_{cmdty}^{site',port} + \sum_{port'} Imports_{cmdty}^{port',port} \\ = NatDemCont_{cmdty}^{port} + \sum_{site} NatTrans_{cmdty}^{port,site'} + \sum_{port'} Exports_{cmdty}^{port,port'} \end{aligned} \quad (Eqn S5.5)$$

Repeated for all ports and transportable commodities.

$$\forall port, cmdty$$

(iv) Rail Border Crossing Balance – similarly to ports, rail border crossing is a key transportation node in the supply chain to deliver exports. Railway freight is only received by national transportation (although technically this is international transportation) since national transport is associated with railway movements, and international transport is associated with shipping vessel movements.

$$\sum_{site} NatTrans_{cmdty}^{site',railX} = NatDemCont_{cmdty}^{railX} + \sum_{site'} NatTrans_{cmdty}^{railX,site'} \quad (Eqn S5.6)$$

(v) National Demand Balance – National demand for a commodity is met by national demand contributions from any port or site. We predominantly investigate steel demand; our model stops after continuous casting to produce semi-finished steel, which would require further downstream processing into the final products. The location of these processing plants is undefined, hence transportation to final steel consumption demand centres is not considered.

$$NatDemand_{cmdty}^{country} = NatDemCont_{cmdty}^{port} + NatDemCont_{cmdty}^{site} + NatDemCont_{cmdty}^{railX} \quad (Eqn S5.7)$$

Repeated for all countries (Ukraine and trading partners) and commodities.

$$\forall country, cmdty$$

Zero-carbon electricity, hydrogen, and ammonia supply

Electricity, H₂ and NH₃ can be supplied from four different sources:

- a) onshore hybrid solar + wind (RE, greenH₂, greenNH₃ - produced at Site);
- b) offshore wind (offRE, offgreenH₂, offgreenNH₃ - produced at OffshoreSite);
- c) hydropower (HP, hydroH₂, hydroNH₃ - produced at HPP (hydropower plant)); and
- d) nuclear power (NP, pinkH₂, pinkNH₃ - produced at NPP (nuclear power plant)).

$$RawMatSup_{elec}^{site} = Supply_RE^{site} + Supply_offRE^{site} + Supply_NP^{site} + Supply_HP^{site} \quad (Eqn S5.8)$$

$$Supply_offRE^{site} = \sum_{OffSite} NatTrans_{offRE}^{OffSite, Site} \quad (Eqn S5.9)$$

$$Supply_NP^{site} = \sum_{NPP} NatTrans_{NP}^{NPP, Site} \quad (Eqn S5.10)$$

$$Supply_HP^{site} = \sum_{HPP} NatTrans_{HP}^{HPP, Site} \quad (Eqn S5.11)$$

The same equations are repeated for H₂ and NH₃.

Production facilities and existing assets

Existing assets are integrated into the model with two binary variables: (i) to control the investment decision to continue/discontinue the use of existing furnaces (on_or_off), and (ii) to enable minimum

capacity determination for any process (install_or_not). Production demand was met by a combination of active existing assets and new assets (NewCap), comprising the total production capacity (TotCap). If existing assets were not utilised, the corresponding furnaces were retired. A distinction is made between furnaces and capacities, to ensure that both binary conditions are met and total production capacity is observed.

$$TotCap_{process}^{site} * f_{util} \geq ProdOut_{process}^{site} \quad (Eqn S5.12)$$

The furnace capacity utilisation factor (f_{util}) of 85% was assumed for all furnaces which was the upper end of observed capacity utilizations over the last 20 years, considered necessary for the industry to make new investments (Vogl et al., 2021b). Although this observation was based on BF-BOF plants, it is considered state-of-the-art for steelmaking and the same assumption will be made for direct reduction and electric furnaces.

$$ActiveExFurnace_{numf,ExFur}^{site} = ExFurnace_{numf,ExFur}^{site} - RetiredFurnace_{numf,ExFur}^{site} \quad (Eqn S5.13)$$

$Numf$ denotes the furnace unit (i.e. furnace number) and $ExFur$ denotes the technology of the existing furnace.

$$ActiveExCap_{process}^{site} = \sum_{numf} \sum_{ExFur} (ExFurnace_{numf,ExFur}^{site} - RetiredFurnace_{numf,ExFur}^{site}) \quad (Eqn S5.14)$$

$$NewCap_{process}^{site} = TotCap_{process}^{site} - ActiveExCap_{process}^{site} \quad (Eqn S5.15)$$

$$\sum_{numf} \sum_{ExFur} ActiveExFurnace_{numf,ExFur}^{site} = \sum_{process} ActiveExCap_{process}^{site} \quad (Eqn S5.16)$$

Retired furnace capacity must be equal to: (i) existing furnace capacity, or (ii) zero (i.e. retire entire facility, not just a fraction of - many inefficiencies occur at partial loads and should be avoided).

$$RetiredFurnace_{numf,ExFur}^{site} = ExFurnace_{numf,ExFur}^{site} * on_or_off_{numf,ExFur}^{site} \quad (Eqn S5.17)$$

New capacity must be equal to: (i) minimum furnace capacity requirement, or (ii) zero. Minimum capacity for processes is 1 Mtpa, excluding EAFs and OSBFs which is set at 0.5 Mtpa.

$$NewCap_{process}^{site} > MinCap_{process} * install_or_not_{process}^{site} \quad (Eqn S5.18)$$

Existing iron and steel production asset data was gathered from the GEM Steel Plant Tracker (GEM, 2022) and GEM Blast Furnace Tracker (GEM, 2023a), including the process capacity, furnace capacities, age of assets and the latest BF relining year.

Production Economics

The overall objective is to minimise the net present value (NPV) of total production, transport, and carbon costs. Production costs are separated into the NPV of OPEX (of all facilities), CAPEX of new assets, CAPEX of active existing capacity that has not yet fully depreciated (i.e. construction year < 20 years ago) and debt incurred due to retirement of assets that have not yet fully depreciated. Transport costs are separated into land transport costs (via railway, pipeline, electricity grid), sea transport costs (via dry bulk carriers and liquefied gas tankers), and the additional processing demands for transporting HBI (briquetting and heating pre-DRI). The price of carbon is also calculated according to the anticipated domestic UA-ETS policy and CBAM on exports to the EU.

$$\begin{aligned} \text{Minimise: } NPV^{sector} = & NPV^{OPEX} + CAPEX^{NewAssets} + CAPEX^{ActiveExCap} + \\ & CAPEX^{BFreline} + Debt^{RetiredAssets} + NPV^{LandTrans} + NPV^{SeaTrans} + \\ & NPV^{HBIburden} + NPV^{CTax} \end{aligned} \quad (Eqn S5.19)$$

The NPV is a sum of all costs over the 20-year project lifetime. The time variable (Y) is introduced for cost parameters that will change over time – renewable electricity, green H₂ and green NH₃ costs, commodity prices, carbon prices, carbon-intensity benchmarks, and reduction factors for free allowances.

A discount factor is applied to calculate the present value of future incurred costs. 2030, 2040 and 2050 are the model start year (Year 0) and the 20 subsequent years are the operation years.

$$df_{OpYear} = \frac{1}{(1 + r)^Y} \quad (Eqn S5.20)$$

The NPV for operational expenditures is defined as:

$$(Eqn S5.21)$$

$$NPV^{OPEX} = \sum_{site} \sum_{comdty} \sum_{Y=1}^{20} (((RawMatSup_{comdty}^{site} * ComPrice_{comdty}^Y) + (CAPEX^{TotAssets} * f_{M\&I})) * df_Y)$$

Where:

$$CAPEX^{TotAssets} = \sum_{site} \sum_{process} (TotCap_{process}^{site} * upCAPEX_{process} * (1 + f_{greenfield}^{site})) \quad (Eqn S5.22)$$

Labour was treated as a commodity. The price of commodities (ComPrice) and unit prices of capital assets (upCAPEX) are detailed in Table X. The cost factor for maintenance and insurance of assets ($f_{M\&I}$) was 4% (Garcia & Berghout, 2019; Wijayanta et al., 2019). An additional 10% economic burden was applied to new sites ($f_{greenfield}$) to account for the cost-benefits of utilising existing human and physical capital in existing (brownfield) sites, for example, a skilled workforce and railway connections to nearby ports. These effects are softened in the context of war where a portion of critical infrastructure has been destroyed and skilled workers have been dislocated; in a non-war context, a 25% capital premium for greenfield projects would be more appropriate.

Logic for existing capacity:

- If utilising existing capacity, pay for any remaining capital payments
- If utilising existing BF capacity, also must account for BF relining
- If not utilising existing capacity, still must pay for any remaining capital payments (debt)

To determine the present value of partly depreciated capital: (Eqn S5.23)

$$CAPEX^{ActiveExCap} = \sum_{site} \sum_{numf} \sum_{ExFur} (ActiveExFurnace_{numf,ExFur}^{site} * upCAPEX_{ExFur} * \frac{f_{CR}}{adj_f_{CR_{numf}}^{site}})$$

$$f_{CR} = \frac{r(1+r)^n}{(1+r)^n - 1} \quad (Eqn S5.24)$$

Where f_{CR} denotes the capital recovery factor, r denotes the real discount rate (8%; 0.08) and n the project lifetime (20 years).

And adj_f_{CR} denotes the adjusted capital recovery factor, which is similarly calculated to f_{CR} yet with n_{adj} which is the remaining payment period related to existing furnaces where capital has not yet fully depreciated (i.e. the furnace was constructed less than 20 years ago). $Y_{construct}$ refers to the year of asset

construction in years (ago) and Y_{reline} refers to the year of BF relining in years (ago), both in reference to the model year (2030, 2040 or 2050).

$$n_{adj_{numf}}^{site} = n - Y_{construct} \quad (Eqn S5.25)$$

$$\text{or, } n_{adj_{numf}}^{site} = n - Y_{reline} \quad (Eqn S5.26)$$

All BFs will require one relining in the 20-year project lifetime; the median historic BF campaign life is 17 years and capital is approximately 40% of the original BF investment (Vogl et al., 2021b). To determine the present value of future BF relining costs (capital and labour), we multiply costs by an adjusted discount factor.

$$NPV^{BFreline} = \sum_{site} \sum_{numf} \sum_{ExFur} \sum_{Y=1}^{20} (ActiveExFurnace_{numf,ExFur}^{site} * \frac{upBFreline + (labourBFreline * ComPrice_{labour}^Y)}{(1 + r)^{n_{adj_{numf}}^{site}}}) \quad (Eqn S5.27)$$

$\forall ExBF$

For debt of required assets, we calculate the present value of partly depreciated capital:

$$Debt^{RetiredAssets} = \sum_{site} \sum_{numf} \sum_{ExFur} (RetiredFurnace_{numf,ExFur}^{site} * upCAPEX_{ExFur} * \frac{f_{CR}}{adj_{f_{CR}}^{site}}) \quad (Eqn S5.28)$$

Natural resource and circularity constraints

(i) Land availability for renewable energy infrastructure (hybrid onshore solar and wind) must be more than the combined land consumption of RE, H₂ and NH₃. Land consumption is determined by the quantity of commodity supplied and land intensity factor of each commodity. The steel sector can only consume 20% of total land availability for solar panels and wind turbines.

$$RELandAvlb^{site} * 20\% > \sum_{RE,H2,NH} (RawMatSupply_{cmdty}^{site} * LandInt_{cmdty}^{site}) \quad (Eqn S5.29)$$

(ii) Sea area availability for offshore wind infrastructure must be more than the combined sea area consumption of RE, H₂ and NH₃. Sea consumption is determined by the quantity of commodity supplied

and sea area intensity factor for each commodity. The steel sector can only consume 20% of available sea area for wind turbine installation.

$$owSeaAvlb^{site} * 20\% > \sum_{RE,H2,NH} (RawMatSupply_{cmdty}^{OffshoreSite} * SeaInt_{cmdty}^{OffshoreSite}) \quad (Eqn S5.30)$$

(iii) Ore reserves and supply

We know the historical output of ore from a mine, characterised by Fe% and the form of the final product (e.g., 65% Fe pellets). However, there is a noticeable lack of information regarding the Fe content at a more granular spatial resolution and the relationship between in-situ ore type and Fe-content, and beneficiation costs. Hence, simplification of ore product costs is employed (BF-grade ore \$80/t and DR-grade ore \$100/t) with constraints on BF-grade and DR-grade ore production capacity.

Ore supply is constrained by annual ore output at a particular mine (AnnualOreOut).

$$AnnualOreOut_{grade}^{mine} > \sum_{site'} NatTrans_{ore_{grade}}^{mine,site'} \quad (Eqn S5.31)$$

Where n is project lifetime (20 years) and mass efficiency considers the mass conversion rate from reserve (extracted material quantity) to final product (65% or 67%-Fe grade ore), therefore taking into consideration the amount of gangue lost in crushing, screening, comminution and beneficiation processes.

No transport of anything other than ore from mines to sites:

$$0 = NatTrans_{cmdty}^{mine,site} \quad \forall cmdty \text{ not } \in ore \quad (Eqn S5.32)$$

No transport of any commodity to mines:

$$0 = NatTrans_{cmdty}^{site,mine} \quad \forall cmdty \quad (Eqn S5.33)$$

(iv) Metallurgical coal and natural gas reserves and supply

The equations for ore mines were adjusted to satisfy metallurgical coal mines (CoalMine) and natural gas refineries (NGRefinery). Strip ratio is not relevant for NG, but refinery efficiency is, which is used to determine an eqv mass ratio; approximately 90% refinery efficiency (Forman et al., 2014).

(v) Scrap steel availability

National scrap steel availability was determined by dynamic material flow analysis, then distributed across sites as a function of population density.

$$ScrapAvlb^{site} > ScrapSupply^{site} \quad (Eqn S5.34)$$

Emissions and imposed carbon prices

Emissions were firstly calculated at site-level using set emission factors (EF) given in Table S.2.11, then aggregated by steel class – primary (ore-based) and secondary (scrap-based). CO₂ emissions are referred to rather than GHG emissions since CO₂ is the primary emission source. Scope 2 emissions were zero since all energy was derived from renewables.

$$TotScope1^{class} = \sum_{site, process} (ProdOut_{process}^{site} * EF_{process}) \quad \forall process \in class \quad (Eqn S5.35)$$

Table S5.23 Scope 1 emission factors for iron and steelmaking processes

	Process	Product	Scope 1 emissions (t CO ₂ /t product)	Reference
Traditional technology	Integrated BF-BOF	LS (total route)	2.400	Metinvest (2020); Koolen (2022)
	coking	coke	0.113	Case with zero-emissions electricity, escalated to 2.410 total emissions (Fan & Friedmann, 2021)
	sintering	ore65sinter	0.304	" "
	BF	pigi	1.931	" "
	BOF	LS	0.050	Reduced relative BOF emissions (transferring to BF) to align with DRI-OSBF-BOF route emission-intensities (MPP, 2022)
Transitional technology	DRI-EAF with 100% NG	LS (total route)	0.560	
	DRIwNG-67o	HBI-C4-67o	0.435	Fig 14 from Müller et al. (2021)
	EAFwDRI-C4	LS	0.146	Vogl et al. (2018); Jacobasch et al. (2021)
	DRI-OSBF-BOF with 100% NG	LS (total route)	0.681	
	DRIwNG-65o	HBI-C4-65o	0.435	Fig 14 from Müller et al. (2021)
	OSBFwDRI-C4	pigi	0.146	Assumed same as EAFwDRI-C4
	BOF	LS	0.050	
	DRI-OSBF-BOF with 70% NG/30% H ₂	LS (total route)	0.496	
	DRIw70NG-67o	HBI-C4-67o	0.367	Fig 14 from Müller et al. (2021)
	EAFwDRI-C4	LS	0.146	

	DRI-OSBF-BOF with 65% H ₂ /35% NG	LS (total route)	0.361	
	DRIw65H ₂ -67o	HBI-C4-67o	0.226	Fig 14 from Müller et al. (2021)
	EAFwDRI-C4	LS	0.146	
Near-zero carbon technology	EAFwscrap	LS	0.099	assuming oxidation of carbon within scrap (~1-2%-C) is approx. average of DRI with 4%-C and 0%-C content; Burchart-Korol (2013) calculated 0.26t CO ₂ /t steel for scrap-based steelmaking in Poland which represents emissions intensive technology rather than BAT
	H ₂ -DRI-EAF	LS (total route)	0.053	
	DRIwH ₂ -67o	HBI-C0-67o	0.000	Vogl et al. (2018)
	EAFwDRI-C0	LS	0.053	Vogl et al. (2018)
	H ₂ -DRI-OSBF-BOF	LS (total route)	0.103	
	DRIwH ₂ -65o	HBI-C0-65o	0.000	Vogl et al. (2018)
	OSBFwDRI-C0	pigi	0.053	Assumed same as EAFwDRI-C0
	BOF	LS	0.050	

There were two separate calculations for carbon prices: domestic carbon tax and CBAM. Only for the 2030 Partial Liberation scenario did Ukraine not have EU membership and therefore CBAM for EU/UK exports was relevant, otherwise, Ukraine's domestic carbon tax was given by the EU-ETS. f_{reduc} denotes the reduction factors for free allowances, which under the EU-ETS, are allocated to trade-exposed industries to prevent carbon leakage.

$$AllowableCO2_Y^{class} = BenchCO2_{int_Y}^{class} * PrimarySFS^{class} \quad (Eqn S5.36)$$

$$TaxableCO2_Y^{class} = \min(TotScope1^{class} - AllowableCO2_Y^{class}, 0) \quad (Eqn S5.37)$$

$$DomesticCTax2_Y^{class} = TaxableCO2_Y^{class} * Cprice_Y^{UA} * (1 - f_{reduc_Y}^{UA}) \quad (Eqn S5.38)$$

$$CBAM_Y^{class} = f_{exp_Y}^{class} * TaxableCO2_Y^{class} * ((Cprice_Y^{EU} * (1 - f_{reduc_Y}^{EU}))) - (Cprice_Y^{UA} * (1 - f_{reduc_Y}^{UA})) \quad (Eqn S5.39)$$

$$NPV^{CTax} = \sum_{class} \sum_{Y=1}^{20} (df_Y * (DomesticCTax2_Y^{class} + CBAM_Y^{class})) \quad (Eqn S5.40)$$

Transport economics

Commodities can be transported nationally using railway freight (dry bulk goods), pipeline (liquefied NH₃, NG) or grids (electricity). The unit cost of dry bulk railway freight in Ukraine is approximately \$0.025 per tonne per km (Forbes, 2022), equivalent to \$0.043/t/km (one-way distance) when the return journey is considered with a 30% fuel consumption reduction on the return leg. Pipeline costs for liquefied NH₃ were taken to be \$0.05/t/km (Nayak-Luke et al., 2021) and NG to be \$0.08/t/km (DeSantis et al., 2021). The Ukrainian National Commission for State Regulation of Energy and Public Utilities (Verkhovna

Rada of Ukraine, 2022) resolved the electricity transmission tariff for green metallurgical enterprises to be \$5.67/MWh/km, a 57% reduction on the generic tariff, which is applied for electricity transportation. A cost uplift of 55% is applied to offshore electricity transmission and liquefied NH₃ pipeline, proportional to the uplift on offshore wind power plants compared to onshore. CGH₂ pipeline for offshore wind plants is costed at \$2/t H₂/km, constrained to a maximum 500km transported distance (Graf, 2021), and CGH₂ by truck freight is costed at \$12.5/t H₂/km (mean of 50km and 300km transmission costs (\$1.875/kg H₂), divided by the transport distance (150km) and expressed in tonnes; data from Yang and Ogden (2007)) and constrained to maximum 150km transported distance – so expensive it is not expected to be utilised. The straight-line distance plus a land margin of 30% was applied to determine the overall transported distance.

$$CostTransLand_{cmdty} = \sum_{loc, loc'} (NatTrans_{cmdty}^{loc, loc'} * LandDist^{loc, loc'}) * (1 + LandMargin) * ucLandTrans_{cmdty} \quad (Eqn S5.41)$$

$$NPV^{LandTrans} = \sum_{cmdty} \sum_{Y=1}^{20} (CostTransLand_{cmdty} * df_Y) \quad (Eqn S5.42)$$

International transportation to facilitate exports from Ukraine to the EU was enabled by dry bulk carriers (DBC) to ship dry bulk goods (SFS, HBI) and liquefied gas tankers (LGT) to ship NH₃ at -33°C. Both vessel categories pertain various sizes and payload capacities; selection is based on importing/exporting port draft and length, and cost-minimisation of vessel journeys considering charter fees, berthing fees, and fuel consumption (cost parameters from Devlin and Yang (2022) and Salmon et al. (2021)). All vessels are assumed to use green NH₃, with the cost determined by the average cost across all sites in the modelled year.

$$TransTonnage_{DBC}^{port, port'} = \sum_{bulk} NatTrans_{DBC, bulk}^{port, port'} \quad (Eqn S5.43)$$

$$\forall DBC, \text{ if: } CarrierDraft_{DBC} < PortDraft^{port, port'} \\ \text{and: } CarrierLength_{DBC} < PortLength^{port, port'}$$

Since charter fees are a daily rate, calculate the number of journeys for each vessel:

$$NumJourneys_{DBC}^{port, port'} = \frac{TransTonnage_{DBC}^{port, port'}}{CarrierPayload_{DBC}} \quad (Eqn S5.44)$$

$$\begin{aligned}
& \text{CostTransSeaBulk}_{DBC,Y}^{port,port'} \quad (Eqn S5.45) \\
& = \text{NumJourneys}_{DBC}^{port,port'} * \text{CarrierCharterFee}_{DBC} * \frac{\text{SeaDist}_{DBC} * \text{SeaMargin} * 2}{\text{CarrierSpeed} * 24} \\
& + (\text{CarrierBerthFee}_{DBC} * 2) + (\text{CarrierFuelCons}_{DBC} * \text{SeaDist}_{DBC} * \text{SeaMargin} * 2 \\
& * ucNH3_Y) + (\text{CarrierPayload}_{DBC} * \text{TurkeyFee})
\end{aligned}$$

Where a sea margin of 15% is applied according to standard shipping provision for increased distance travelled due to factors including high winds, currents, and shallow water (Wärtsilä, 2023). *TurkeyFee* is the additional fee of \$4/t cargo applied to all routes that pass by Turkey's Bosphorus and Dardanelles (GMK, 2023b).

A very similar set of equations was utilised to calculate international transportation costs using LGTs, then NPV determined for total sea transportation costs:

$$NPV^{SeaTrans} = \sum_{port} \sum_{port'} \sum_{DBC} \sum_{Y=1}^{20} ((\text{CostTransSeaBulk}_{DBC}^{port,port'} + \text{CostTransSeaLiq}_{LGT}^{port,port'}) * df_Y) \quad (Eqn S5.46)$$

To calculate the additional cost burdens for HBI briquetting and HBI heating pre-DRI that would not be incurred if iron and steelmaking were co-located, we use the following equations:

$$\text{CostHBIBriq}_Y^{loc,loc'} = \text{NatTrans}_{HBI'}^{loc,loc'} * \text{ElecPrice}_Y^{loc} * \text{ElecCons_Briq} \quad (Eqn S5.47)$$

$$\text{CostHBIheat}_Y^{loc,loc'} = \text{NatTrans}_{HBI'}^{loc,loc'} * \text{ElecPrice}_Y^{loc'} * \text{ElecCons_HBIheat} \quad (Eqn S5.48)$$

$\forall \text{ not Colocation}(loc, loc')$

$$NPV^{HBIBurden} = \sum_{loc} \sum_{loc'} \sum_{Y=1}^{20} ((\text{CostHBIBriq}_Y^{loc,lo} + \text{CostHBIheat}_Y^{loc,loc'}) * df_Y) \quad (Eqn S5.49)$$

For the cost of HBI heating pre-DRI the electricity price of the importing site/country is applied, whereas for HBI briquetting the electricity price of the exporting country is applied.

Figure S5.18 Modelled steel production routes in the green steel transition study. Minor inputs, including oxygen, alloys, and fluxes, are not shown for simplicity. Transportable commodities are classified into three types: (i) local (loc): transport only within same grid (1°x1°); (ii) national (nat): transport within national borders, and; (iii) exportable (exp): transport both within national borders, and exportable to other countries.

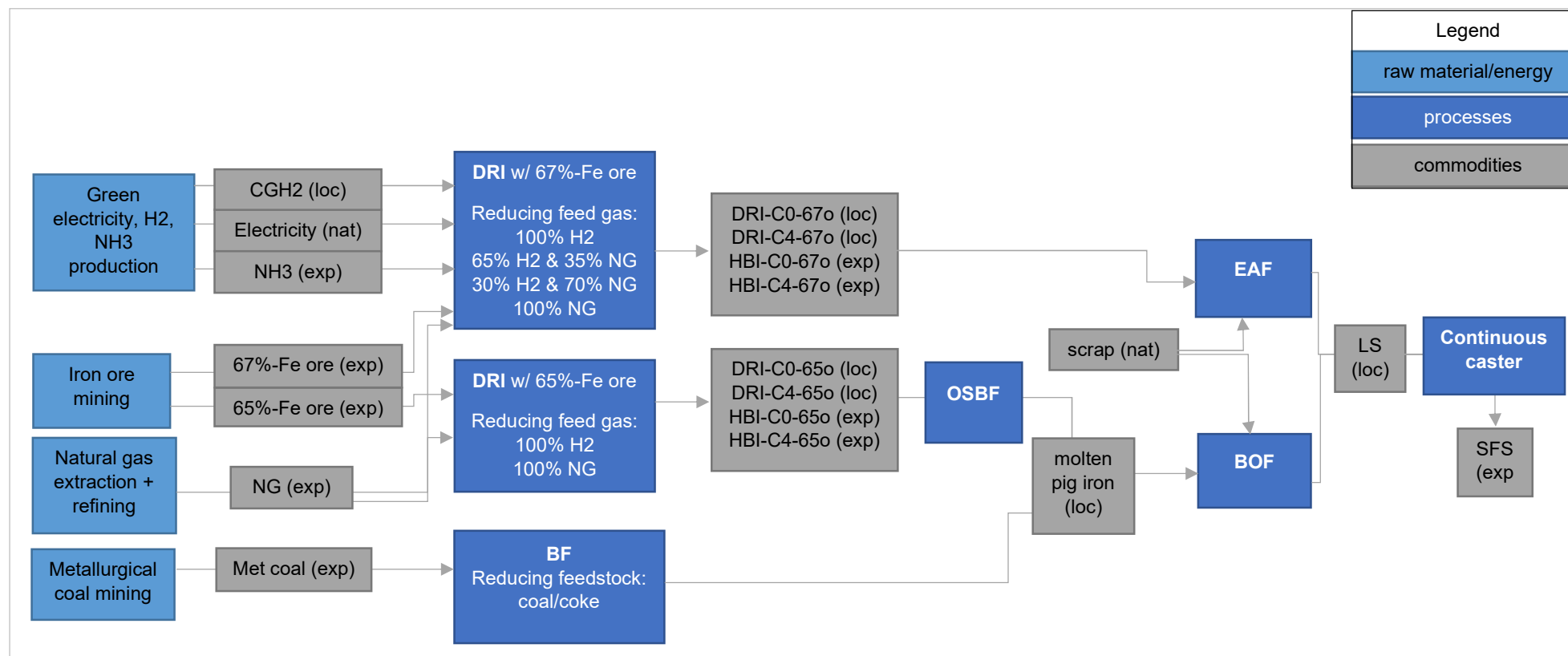


Table S5.24 Specific process consumption rates

	Source→	(Jacobasch et al., 2021; Müller et al., 2021)				(Cavaliere et al., 2022)				(Jacobasch et al., 2021; Müller et al., 2021)		(Kirschen et al., 2011; Vogl et al., 2018)	(Giddey et al., 2017)	(IEAGHG, 2013)			(Li et al., 2020)
Process → Input product ↓	Unit ↓	DRIwH2-67o	DRIwNG-67o	DRIw65H2-67o	DRIw70NG-67o	DRIwH2-65o	DRIwNG-65o	OSBFwDRI-C0	OSBFwDRI-C4	EAFwDRI-C0	EAFwDRI-C4	EAFwscrap	Cracking	BF	BOF	Sintering	Coking
ore65pel	t/t product	0	0	0	0	1.437	1.4	0	0	0	0	0	0	0.358	0	0	0
ore65lump	t/t product	0	0	0	0	0	0	0	0	0	0	0	0	0.128	0	0	0
ore65fines	t/t product	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.792	0
ore65sinter	t/t product	0	0	0	0	0	0	0	0	0	0	0	0	1.142	0	0	0
ore67pel	t/t product	1.395	1.36	1.365	1.362	0	0	0	0	0	0	0	0	0	0	0	0
elec	MWh/t product	0.083	0.083	0.083	0.083	0.113	0.113	0.66	0.66	0.518	0.47	0.657	0.29	0	0.01	0	0.045
NH ₃	t/t product	0	0	0	0	0	0	0	0	0	0	0	6.667	0	0	0	0
H ₂	t/t product	0.067	0	0.028	0.006	0.067	0	0	0	0	0	0	0	0	0	0	0
NG	t/t product	0	0.208	0.121	0.189	0	0.208	0	0	0	0	0	0	0	0	0	0
metcoal	t/t product	0	0	0	0	0	0	0	0	0	0	0	0	0.155	0	0	1.32
coke	t/t product	0	0	0	0	0	0	0	0	0	0	0	0	0.362	0	0	0
HBI-C0-65o	t/t product	0	0	0	0	0	0	1.15	0	0	0	0	0	0	0	0	0
HBI-C0-67o	t/t product	0	0	0	0	0	0	0	0	0.846	0	0	0	0	0	0	0
HBI-C4-65o	t/t product	0	0	0	0	0	0	0	1.15	0	0	0	0	0	0	0	0
HBI-C4-67o	t/t product	0	0	0	0	0	0	0	0	0	0.924	0	0	0	0	0	0
pigi	t/t product	0	0	0	0	0	0	0	0	0	0	0	0	0	0.869	0	0
scrap	t/t product	0	0	0	0	0	0	0	0	0.194	0.194	1.02	0	0	0.118	0	0
lime	t/t product	0	0	0	0	0	0	0.0114	0.0114	0.05	0.053	0.029	0	0	0.068	0.01	0
limestone	t/t product	0	0	0	0	0	0	0	0	0	0	0	0	0.013	0	0.117	0
alloys	t/t product	0	0	0	0	0	0	0	0	0.011	0.011	0.011	0	0	0.015	0	0
oxygen	t/t product	0	0.086	0.057	0.076	0.079	0.079	0	0	0.004	0.056	0.045	0	0.07	0.071	0	0
carbon	t/t product	0	0	0	0	0	0	0.01	0	0.01	0	0.01	0	0	0	0	0
electrode	t/t product	0	0	0	0	0	0	0.003	0.003	0.002	0.002	0.002	0	0	0	0	0
refractory	t/t product	0	0	0	0	0	0	0	0	0.005	0.005	0.005	0	0	0.005	0	0
labour	t/t product	5	5	5	5	5	5	1	1	1	1	1	0	3	2	1	2
Output product		HBI-C0-67o	HBI-C4-67o	HBI-C4-67o	HBI-C4-67o	HBI-C0-65o	HBI-C4-65o	pigi	pigi	SFS	SFS	SFS	H ₂	pigi	SFS	ore65sinter	coke

Table S5.25 Commodity prices and labour costs (excluding zero-carbon energy products)

	Value	Unit	Source
DR-grade ore	100	\$/dmt	based on costs from Black Iron (2023)
BF-grade ore	80	\$/dmt	World Bank Group (2022a)
Scrap	300	\$/t	GMK (2021)
Natural gas	25	\$/MWh	Eurostat (2023)
Metallurgical coal	200	\$/t	(\$196 = 5-yr avg 2018-2022) Department of Industry (2023)
Lime	121	\$/t	Vogl et al. (2018)
Limestone	11	\$/t	Author's estimate
Alloys	2397	\$/t	Vogl et al. (2018)
Oxygen	82	\$/t	Vogl et al. (2018)
Carbon	300	\$/t	premium for anthracite above metallurgical coal
Electrodes	5395	\$/t	Vogl et al. (2018)
Refractories	1100	\$/t	Deneen and Gross (2010)
Water	2	\$/t	-Bryan Municipal Utilities
Labour	3	\$/hr	based on costs from Black Iron (2023)

Table S5.26 Unit Prices of iron and steelmaking assets

Asset	Value	Unit	Source
coke plant	268	\$/tpa coke	IEAGHG (2013)
sinter plant	56	\$/tpa sinter	IEAGHG (2013)
BF	225	\$/tpa pig iron	IEAGHG (2013)
BOF	120	\$/tpa LS	IEAGHG (2013)
BF reline	100	\$/tpa pig iron	Teck (2022)
EAF	283	\$/tpa LS	Vogl et al. (2018), Facchini et al. (2021), (Steelonthenet.com, 2022)
OSBF	283	\$/tpa LS	<i>assume same as EAF, both electric smelting furnaces</i>
DRI shaft furnace	310	\$/tpa DRI	Vogl et al. (2018)
NH ₃ cracker	30	\$/tpa NH ₃	Cesaro et al. (2021)

Economic multiplier analysis

The macroeconomic analysis was conducted on the historical basic metals industry, based on data published by the Ukraine State Statistics Service (1990-2021), which provided complete flows of products (goods and services) in the economy for a given year. Since 2015, data has been produced on total use of domestic production at basic prices disaggregated into intermediate consumption by 42 industries/products (NACE Rev. 2) and seven final demand sectors, including final consumption expenditure (of households; non-profit institutions services households; general government), gross capital formation (including gross fixed capital formation; changes in inventories; and net acquisition of valuables), and exports of goods and services. These I-O Tables denote the relationship between producers and consumers and the interdependencies of domestic industries.

To generate output multipliers, firstly, the initial monetary values in the transaction matrices were converted into ratios called technical coefficients, by dividing each cell of the domestic intermediate matrix by its column total (output at basic prices). These technical coefficients can be used directly to access the added value of a given sector (e.g., see Table S5.9 for the dataset on domestic outputs of the basic metals industry). Consequently, to calculate the output multipliers, Leontief Inverse matrices were derived, which show for each industry the direct and indirect (Type I), and direct, indirect, and induced (Type II) effects upon the total output of an additional 1-unit of currency (UAH, Ukrainian hryvnia) of final demand. Income and GVA multipliers were subsequently derived using the standard matrix algebraic formulas. We have not produced employment multipliers because employment numbers coherent with the Ukrainian balanced compensation of employee's data have never been published by the Ukraine State Statistics Service.

Secondly, the macroeconomic impact of the optimised future green steel sector was modelled for national output, income, and GVA patterns, using Type I and Type II standard multipliers and effect multipliers. For comparison, the economic impact of the same magnitude of steel production under traditional coal-based steel scenarios were assessed, based on the latest pre-war (i.e., 2021) Type II output multipliers, and the corresponding income and GVA effects by simply inputting the value of steel in US\$ to be produced by the basic metals industry. The expenditure of green steel scenarios was broken down into the industry's key intermediate production suppliers and output multipliers used to determine output, income, and GVA impacts, then their backward and forward linkages determined as 'extra' output, income, and GVA. The sum of which provided an approximate indication of the macroeconomic effects associated with the new green steel production function. For the green scenarios, whilst inputs and expenditure are redefined, historical I-O multipliers from 2021 must still be employed as the most recent data available.

The green steel assessments were based on conservative assumptions, with avoidance of double counting of outputs generated by the industry suppliers. For GVA forecasts, the average gross operation surplus was assumed to be 8%, despite the fact that over the last decade, international steel industry's earnings before interest, taxes, depreciation, and amortisation - EBITDA margins – have averaged 8-10% (McKinsey&Company) . The green steel analysis is primarily conducted for the full liberation of Ukraine with greater steel demand – the macroeconomic benefits of the *Slow Recovery* scenario are, on average, half that of the *Strong Recovery* scenario.

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