Development of a Novel ‘Hub & Spoke’ Framework for the Holistic Sustainability Assessment of Fast-Moving Consumer Goods Oriented Value Chains

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Doctor of Philosophy

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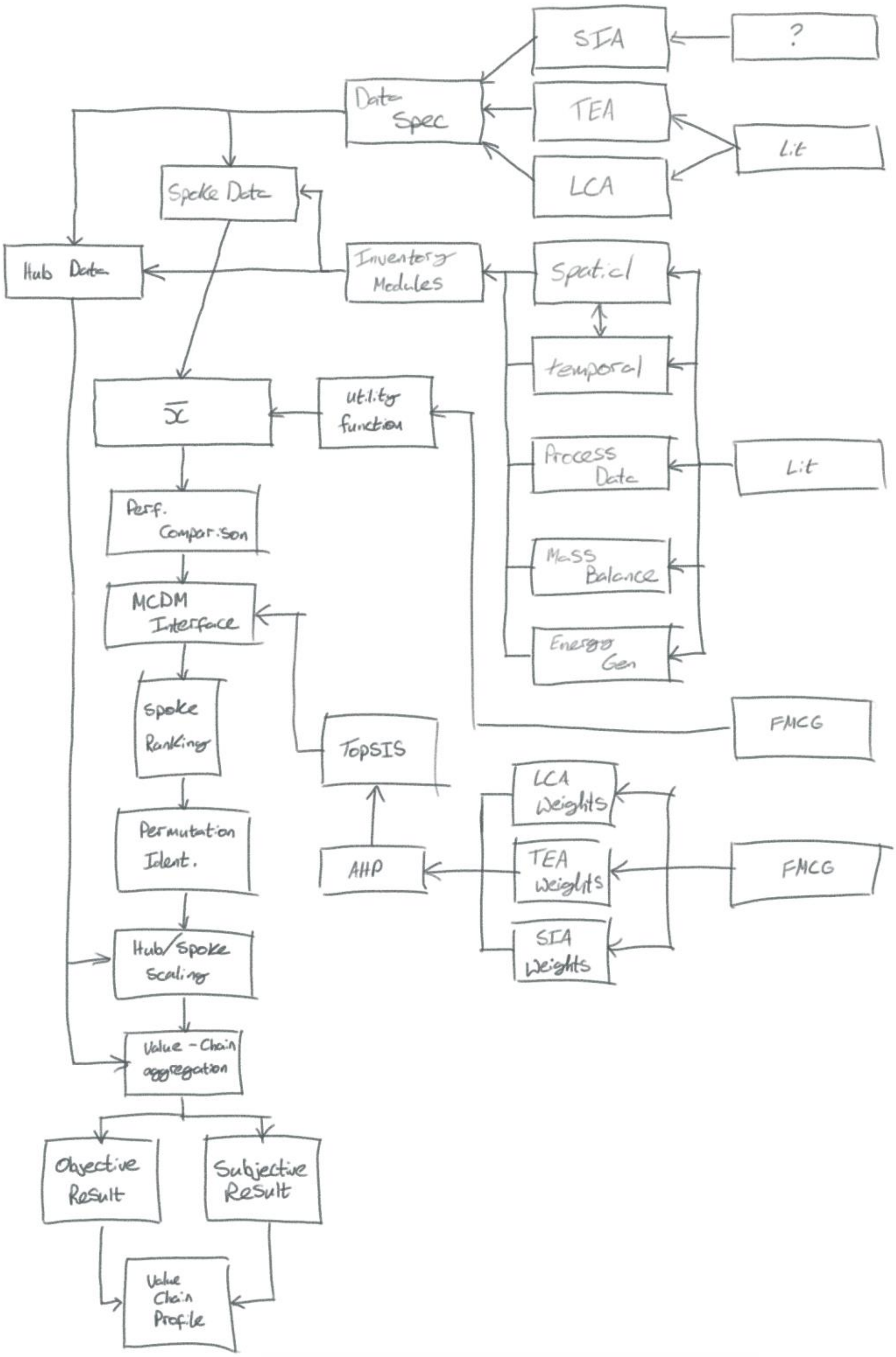
TINGITUR ANIMA COLORE COGITATIONUM

Marcus Aurelius c. 150 A.D.



A scan of the first notebook sketch of what went on to become the framework architecture that forms the backbone of this PhD project. Drawn sometime in the early hours of a non-descript October morning, 2022 (one of the only notebook musings I didn't think to date).

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<u>Personal</u>

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Our motto is as pertinent today as when we were founded in 1905…

"Rerum Cognoscere Causas"
(To discover the causes)

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Abstract

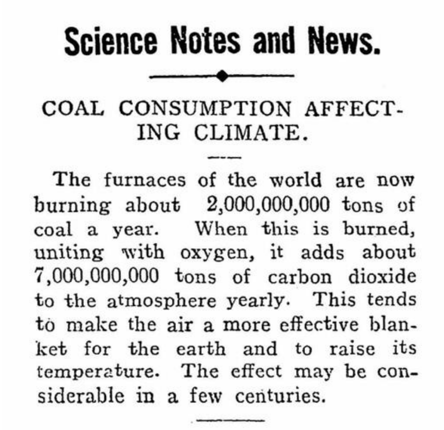
Many critics of 'big industry' perceive the idea of sustainable corporate strategy to be inherently oxymoronic, particularly in sectors such as fast-moving consumer goods, where high production volumes and resource-intensive supply chains contribute significantly to global environmental challenges. The work herein aims to counter this ideology, developing a fast-moving consumer goods value chain oriented holistic sustainability assessment methodology. Through this approach, the commissioning organisation's strategy or values are also directly incorporated. Sustainability in fast-moving consumer goods (environmental, economic, and social) is particularly complex due to the sector's reliance on resource extraction, energy-intensive manufacturing, and extensive logistics networks. Carbon dioxide utilisation has emerged as a potential strategy to reduce industrial emissions by transforming CO_2 waste into valuable products, offering a promising pathway toward circularity in industrial operations. However, existing sustainability assessment frameworks often fail to comprehensively account for the integration of carbon dioxide utilisation within fast-moving consumer goods value chains.

Several key gaps in historic capability are first identified via literature review (data architecture and social impact characterisation methods). The closure of these was deemed necessary for the attainment of an efficacious framework; meaningfully integrating environmental, economic, and societal assessments. To rectify these shortcomings a novel 'hub and spoke' methodological architecture is developed, delivering objective (practitioner oriented) and subjective (industrial decision maker oriented) results streams. The objective results are comparable to those seen in existing environmental and economic studies, with the addition of first of their kind quantitative and repeatable social indicators. In contrast, the subjective results are derived through the parallel application of multicriteria decision making techniques, delivering a single overall score for each considered value chain permutation. To fully align the social strand with its environmental and economic counterparts, new impact pathway-based characterisation models are developed, covering seven United Nations endorsed indicators across 129 countries. These two methodological developments are then evaluated for efficacy through a proof-of-concept study, examining soda ash production in India.

The framework was used to examine Hou process based soda ash production in the Asia and Pacific region, delivering cradle-to-gate holistic sustainability profiles for 14,580 unique value chain permutations while assessing a total of 19 impact indicators. As the most commonly assessed indicator, accuracy of the framework's results generation procedure was verified through comparison of the average global warming potential value across the assessed permutations to literature value; specifically, industry average values for the Hou process extracted from the Ecoinvent database. This revealed a negligible 0.72% difference between the hub and spoke framework's result (2.77 tonnes CO_2-eq. per tonne of soda ash) and the literature value (2.79 tonnes CO_2-eq. per tonne soda ash). Opportunities for significant impact reductions were also identified, although these are realised at the expense of other indicators. Again, using global warming potential as an example, a potential 91.1% emission reduction scenario is identified (0.25 tonnes CO_2-eq. per tonne soda ash), utilising a direct air capture CO_2 feed, with biogas combustion and electricity supplying process energy. Overall, the hub and spoke framework was shown to effectively rank large numbers of value chain alternatives based on their objective performance, as well as the value choices prescribed by industrial decision makers. Consequently, this work is deemed to present a notable step towards operationalising holistic sustainability assessment both within, and beyond, practitioner audiences.

1 Introduction

As early as 1912, news outlets and select mining journals began to blow the proverbial whistle on global coal usage and the associated effects on our planet's fragile atmosphere (Figure 1-1). The global turmoil experienced in the following few decades did much to quiet calls for awareness and action. This failure to recognise the scope of the problem has resulted in a 50% rise in atmospheric CO_2 concentration since the beginning of the industrial revolution (c. 1760) [1]. In efforts to measure and understand this rise, the U.S. based National Oceanic and Atmospheric Administration began accurately measuring atmospheric CO_2 concentration in 1958 at the Mauna Loa Observatory, Hawaii. More recently, data from NASA's Atmospheric Infrared Sounder (AIRS) has shown a 19% rise in average annual concentration over the two decades between 2002 and 2022 [2], confirming an increasing rate of accumulation. In recognition of this, climate scientists have proposed that humanity has forced the Earth out of the Holocene, the period that nurtured societal development, and into a proposed Anthropocene epoch; one in which human activities now rival geological forces as the main climate driver, directly altering the planets conditions [3]. The resulting impacts will, if no meaningful action is taken, significantly alter climates and societies.


Science Notes and News.

COAL CONSUMPTION AFFECTING CLIMATE.

The furnaces of the world are now burning about 2,000,000,000 tons of coal a year. When this is burned, uniting with oxygen, it adds about 7,000,000,000 tons of carbon dioxide to the atmosphere yearly. This tends to make the air a more effective blanket for the earth and to raise its temperature. The effect may be considerable in a few centuries.

Figure 1-1 – Extract from the Braidwood Dispatch and Mining Journal [4]

A significant milestone was reached on 22nd April 2016 with the signing of the Paris Agreement. With 195 signatory counties, the legally binding agreement focusses on the mitigation and abatement of greenhouse gas (GHG) emissions. The primary goal is: "holding the increase in the global average temperature to well below 2°C above pre-industrial levels and pursuing efforts to limit the temperature increase to 1.5°C above pre-industrial levels, recognising that this would significantly reduce the risks and impacts of climate change" [5].

With both governmental and public awareness of climate change reaching all-time highs, it is critical that organisations adapt to meet evolving societal expectations around planetary stewardship. With ambitious emission reduction targets looming, and no clear path to meeting the Paris Agreement's goals [6], industrial leaders of the future must develop the tools and understanding required to navigate these treacherous, and warming, waters. The increasing interest in, and deployment of, carbon taxation by governments will likely make the use of virgin fossil resources economically uncompetitive. Consequently, the selection and development of responsible value chains should be of the utmost priority. In addition, public perceptions of industrial sustainability have already resulted in significant business pressures. Many consumers are less willing to support or buy from organisations that are not seen to be environmentally progressive, incentivising many companies to address their emissions and wider operational impacts.

We have, as a society, arrived at a critical turning point; one where governments, consumers, and industry, must continue to work symbiotically towards the common goal of limiting emissions and global temperature rise. The scientific community is unsure exactly where a potential tipping point or 'planetary threshold' may be located, beyond which warming will be almost impossible to halt. This scenario is referred to as a "Hothouse Earth". It occurs when natural positive feedback loops are activated, where rising CO_2 levels begin to trigger events that lead to even greater releases. A cascading series of these events may put the planet's climate on an irreversible trajectory [3]. The likelihood of this occurring will significantly increase if a rise of 2°C or more is allowed to occur. Clearly, to meet internationally agreed targets, significant additional changes are needed from policy makers and industry leaders worldwide.

1.1 The Triple Bottom Line

While the mitigation of the environmental impacts associated with anthropogenic activities have been targeted for some time, the issue runs much deeper. Coined by John Elkington, an authority on corporate sustainable development, the triple bottom line is an accounting framework that simultaneously examines the environmental, economic, and social impacts of organisations (summarised in Figure 1-2). This broader approach to sustainability has been adopted within the academic community, resulting in attempts at the development of holistic sustainability assessment techniques; a pertinent example is McCord, *et al.*'s triple helix framework, suggesting that environmental, economic, and social impacts form the three 'strands' of an overall assessment [7]. However, this work is far from complete, currently lacking both repeatability and consensus on best practices.

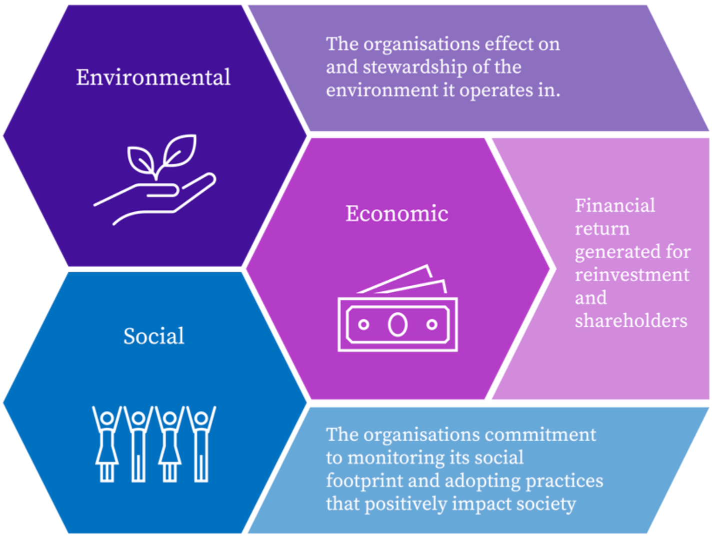


Figure 1-2 – Summary of the triple bottom line.

The framework's value lies in its recognition that environmental, economic, and societal sustainability are intrinsically linked. Environmental impacts, if left unchecked, will worsen as years pass, causing impacts in the other areas. For example, multi-breadbasket failures are highly likely, including wheat, maize and soyabeans [8]; leading to catastrophic food shortages worldwide. Rising sea levels and desertification could lead to the loss of 1.79 M km^2 of land, including critical agricultural regions [9], resulting in approximately a billion 'environmental migrants' by 2050 [10]. Increasing oceanic CO_2 uptake leads to acidification and decreasing dissolved oxygen concentration. This along with other factors has resulted in the projection that by 2050 the catch potential of the world's fisheries could decrease by up to 12.1% [11], compounding the impact of potential breadbasket failures mentioned previously.

1.2 Unilever's 'Clean Future' Initiative

In late 2020 the United Kingdom government set a new target of 68% reduction in GHG emissions by 2030 (relative to 1990 levels); this replaces the previous target of a 53% reduction. As of 2019, total UK GHG emissions were down 45.2% relative to 1990 [12], leaving a further 22.8% reduction required over the course of this decade. This target is reenforced by the Ex-Prime Minister's (Boris Johnson) 'Ten Point Plan for a Green Industrial Revolution', announced in November 2020, including investment within offshore wind, low carbon hydrogen and carbon capture and utilisation (CCU) [13]. The ultimate goal within the UK is the attainment of net zero emissions by 2050 (as opposed to the previous 80% reduction), a target which is now legally binding under the recently amended Climate Change Act, originally penned in 2008 [14] [15].

In response to the climate crisis, as well as societal and legislative pressure, Unilever Homecare unveiled it's 'Clean Future' initiative. Through this, the organisation aims to eliminate all fossil carbon from their homecare formulations by 2030, instead targeting the use of renewable, captured or recycled alternatives, reaching carbon neutrality by 2039:

> "*Through Clean Future, we aim to replace 100% of the carbon derived from fossil fuels in our Home Care formulations with renewable or recycled carbon by 2030*" [16].

This announcement challenged the status quo within the fast-moving consumer goods (FMCG) industry, which generally sources bulk chemicals from archaic and emission intensive processes and value chains. Within the initiative the various sources of carbon are classified by colour, termed the 'carbon rainbow' (Figure 1-3); purple denotes CO_2 derived carbon, blue for marine sources, green for bio-based, and grey from plastic waste [16]. It should be noted that there is a secondary purple arrow originating from production and terminating at carbon processing into useful materials. This represents the capture and utilisation of industrial emissions and will likely be a key factor in reaching a zero-fossil carbon scenario.

While the 'Clean Future' initiative places significant importance on the reduction of GHG emission within Unilever's value chains it also aims to drive improvement in other FMCG relevant areas of environmental sustainability. Two key examples are water and resource depletion. Most food and beverage, textile, and cosmetics value chains require large amounts of process water, potentially contributing to local water stress, particularly in regions already experiencing scarcity. Resource depletion is also of concern to FMCG companies as they rely heavily on a broad range of raw materials including petroleum-based plastics, metals, agricultural commodities, and rare minerals. Reducing the amount of these resources required in products, or finding circular sourcing options, is crucial to maintaining existing product portfolios into the future. Additionally, eutrophication potential is a highly relevant environmental impact in the FMCG sector. The industry's extensive reliance on agriculture, chemical manufacturing, and wastewater-intensive processes has the potential to result in the release of excess nutrients, primarily nitrogen (N) and phosphorus (P), into aquatic ecosystems, leading to oxygen depletion, algal blooms, and biodiversity loss.

A key secondary goal within the initiative, touched upon in the previous discussion of resource depletion, is the shift from linear to circular value chains. By designing value chains that make use of waste products or pollution, our dependence on virgin feedstocks (including carbon) may be reduced significantly. "The circular economy gives us the tools to tackle climate change and biodiversity loss together, while addressing important social needs" [17]. Beyond the environmental and social benefits of circular value chains, the economic value embedded within the 'waste' materials in not lost. If these materials can be valorised without significant processing costs, there are significant financial gains to be realised. Adoption of the principle can be approached through technical cycles, biological cycles, or a combination of the two. The scope of this work focusses on the utilisation of technical cycles, more specifically, the conversion of purple, CO_2 derived, carbon into value added products. Purple sources are less diverse than the other types within the carbon rainbow, primarily resting upon the monoethanolamine (MEA) based point-source, or direct air capture, of CO_2; consequently, they fall under the larger umbrella of carbon dioxide utilisation (CDU).

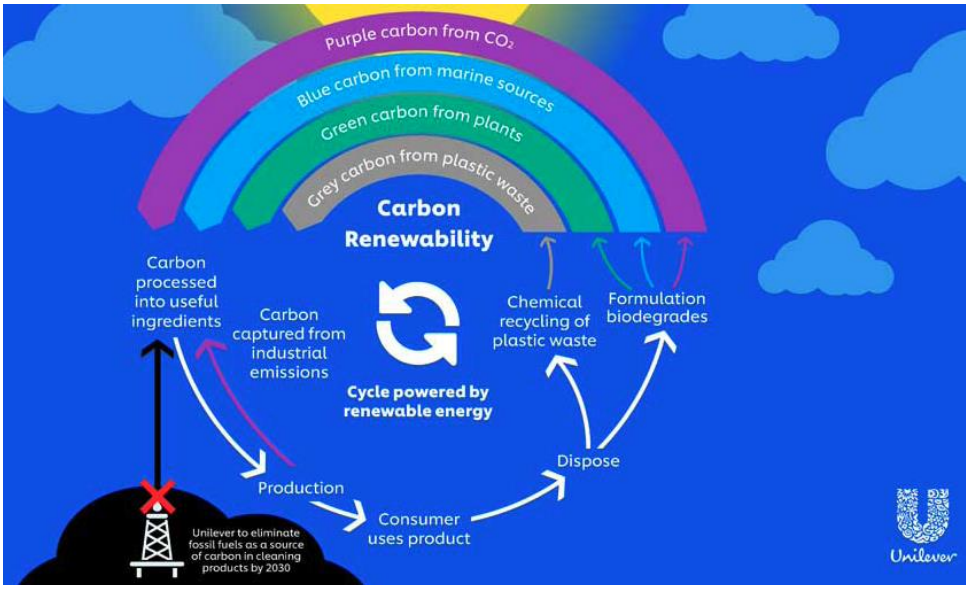


Figure 1-3 – The carbon rainbow, a key part of Unilever's Clean 'Future' Initiative [16].

1.3 Fast Moving Consumer Goods Value Chains

FMCG companies typically necessitate value chains that are both long, and broad. They span various lifecycle phases connecting the consumer to original raw material extraction, including but not limited to; production, distribution, marketing, and retail. FMCG companies therefore look to simplify and expedite the pace of these value chains through optimisation and streamlining. In parallel, fast and dynamic responses to external forces or drivers are crucial in a sector with such short shelf-lives and high rate of demand. With product formulations evolving regularly, new approaches to the mapping and evaluation of value chain nodes are needed.

While products will always pass through factories, warehouses, and onto shelves, FMCG companies will be looking to minimise negative impacts and optimise cost efficiency. With products that often require large numbers of feedstock materials, FMCG companies operate some of the longest and most complex value chains; these must consider, and cater to, the needs and wants of suppliers, manufacturers, distributors, retailers, and customers. From these parties, suppliers and consumers have the largest leverage over these systems due to their terminal positions; consequently, value chain development should consider them carefully. For consumers this means meeting, and communicating compliance with, their needs and values. In terms of suppliers, partnerships must be carried out to maximise performance across economic, environmental, and social metrics. The threshold for acceptable supplier behaviours is often dictated by consumers, a recent phenomenon that originates from their increased awareness of sustainability issues.

With strategic partnerships being commonplace in FMCG research and development (R&D) efforts, rapid sustainability assessment of technologies and their potential integration within value chains is of paramount importance; successful partnership agreements may deliver significant performance gains relative to competitors. These gains can be realised in any of the three strands of sustainability, not just economic. What is clear is that FMCGs value chains require a nuanced and tailored approach to sustainability assessments. With a high degree of decentralisation of control, and a growing number of alternate solutions to every question, an application specific framework is needed to support both sustainability assessment practitioners and industrial decision makers within organisations.

1.4 Current State of Sustainability Assessment

As previously discussed, sustainability goes beyond purely environmental assessment; rather, it can be viewed as a multi-faceted problem with three distinct yet interconnected aspects. The field of sustainability assessment has experienced rapid growth since the turn of the millennium. This is linked to the increasing investment in, and societal shifts towards, the responsible sourcing of goods, services, and chemicals feedstocks. The publication rate within independent assessment strands gives useful insights into the methodologies' maturity and perceived utility. Data for Figure 1-4 was collated using a Web of Science literature search of publication years between 2000 – 2021. Searches required either the full assessment name or abbreviation listed as a keyword (e.g. Lifecycle Assessment or LCA). This returned a total of 110,556 publications. Review papers are not excluded from the publication count, owing to the aim of demonstrating increased interest rather than quantifying evaluations of novel technologies. A full analysis of the state-of-the-art in sustainability assessment is presented in Chapter 3, focussing on CDU (purple carbon).

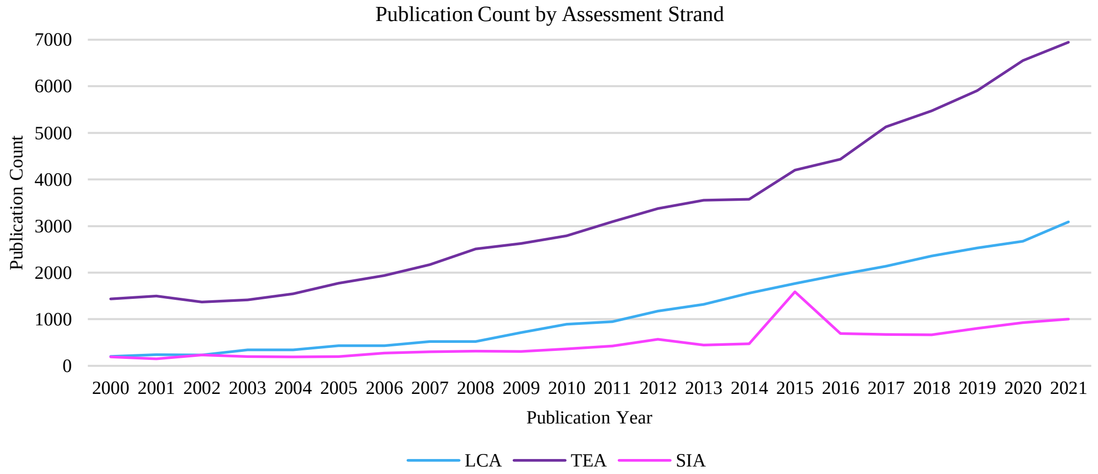


Figure 1-4 - Number of publications listing each independent assessment type or its abbreviation as a keyword, collated by year. Data collected using Web of Science

Examining the results, large bodies of work can be seen around each aspect of sustainability in abstraction. Life Cycle Assessment (LCA), the oldest of the three strands, emerged in the 1960s [18]. Early applications generated what would nowadays be considered partial LCAs, following comparative approaches with no broadly accepted methodology [19]. In 2006, ISO released the 14K series of standards [20], introducing a rigorous and repeatable four phase approach to assessments: goal and scope definition, inventory generation, impact analysis, and interpretation. Despite further development upon ISO's offering, through the ILCD handbook [21], carbon dioxide utilisation specific guidance proved elusive until the GCI (Global CO_2 Initiative) published guidelines specific to the sector in 2018 [22] (succeeded by a second iteration in 2022 [23]). Formal guidance considering the holistic sustainability assessment of FMCG value chains is currently absent from literature.

Consulting Figure 1-4 once again, LCA publications can be seen to grow from an 11% share of sustainability assessment publications to 28% between 2000 and 2021. This can likely be explained by a growing emphasis on environmental protection within the period. It is believed that this was partially catalysed by widely reported upon studies from bodies such as IPCC and the World Meteorological Organisation, revealing record high annual and decadal temperatures [24] [25]. International treaties such as the Paris Agreement added additional legislative pressure internationally [26], further incentivising industry to quantify and reduce their impacts through LCA reporting.

Techno-economic assessment (TEA) is historically less standardised than LCA, lacking a broad consensus on best practices [27] [28]. The variation in approaches observed delivers assessments based on diverse methodological underpinnings and, on occasion, overly optimistic assumptions such as unconstrained supplies of green electricity of hydrogen. However, this did not prevent the publication of large numbers of studies, as shown by Figure 1-4; a consequence of the significant importance of economic insights within industrial decision making. The GCI approached the TEA standardisation problem through the adoption of the now mainstream four phase assessment structure, originally proposed within ISO 14040 [20]; forming CDU oriented guidelines aligned with those developed previously for LCA [22]. When observing Figure 1-4, TEA sees a drop in its relative share of sustainability assessment publications, falling from 79% in 2000 to 63% in 2021.

The third societal strand, social impact assessment (SIA), or social-LCA (S-LCA), maintains a 10% share of sustainability assessment publications between 2000 - 2021; stagnating in its infancy relative to both LCA and TEA [29] [30] [31] [32] [33]. This can reasonably be attributed to its comparatively recent first literature appearance in 1996 [34], making it LCA's junior by approximately three decades. Many organisations evaluate and report social impacts using the Global Reporting Initiative (GRI) standards [35] or UN Sustainable Development Goals (SDGs) [36]. While a valuable starting point, these approaches lack the system-oriented approach seen within LCA and TEA. To rectify this shortcoming, the United Nations Environment Programme (UNEP) and the Society of Environmental Toxicology and Chemistry (SETAC) jointly developed general guidelines for SIA. Despite adopting an ISO derived structure, many discrepancies persist between SIA and LCA, most notably the lack of impact characterisation methods [19]. No standards or guidelines are present for CDU or value-chain oriented application, leaving a single framework (the triple helix framework developed by McCord, *et al*. [7]), intended for implementation alongside the Global CO_2 Initiative (GCI) LCA and TEA guidelines [7].

1.5 Sustainability Assessment's Value Addition to Fast moving Consumer Goods Companies.

In order to provide FMCG companies with a suitable tool through which they can assess new potential value chains, or retrofits to those already deployed, a truly application specific and holistic framework is required. This includes further methodological harmonisation of assessment strands, moving beyond that which was achieved within the triple helix framework, as well as identification of the unique needs of FMCG companies. While recognition of such an approach is not in itself novel, being suggested for other industries from 2007 onwards [37] [38], developmental efforts have stagnated. The improved harmonisation of CDU relevant methodologies, and increased practicality of application, offers a powerful tool in the transition towards sustainable industrial ecosystems and widespread utilisation of purple carbon by FMCG companies.

Through consultation of both academic and corporate literature, several key capabilities are identified that are believed will unlock significant FMCG relevant utility within sustainability assessments. Such insights were previously out of reach within less application specific frameworks. The areas of focus include the ability to evaluate very large numbers of competing value chain permutations, tailoring of recommendation to organisational needs, modular inter-operability of constituent lifecycle inventories, and results communicability to non-practitioner audiences (be that corporate decision makers or consumers). The vast number of feedstock production routes and suppliers make the traditional approach to comparative assessments ineffective and time consuming; a more streamlined approach is therefore necessary if changes to industrial value chains are to be efficacious.

1.6 Thesis Structure

The aims and objectives for this doctoral project lend themselves to stratification and therefore are defined in a hierarchical manner. In this, each chapter is prescribed a core objective which is then divided further into sub-objectives at the beginning of each chapter. It is hoped that this approach helps to deliver a more transparent and compelling narrative; sequentially examining the decisions made, and methods selected, at each stage of framework development. In addition, the two levels of granularity presented through the tiered objective structure allows for more meaningful discussion, facilitating the convenient evaluation of the framework's macro- and micro-level efficacy.

Chapter two, after the setting of research aims and objectives, charts a comprehensive literature review conducted around CDU oriented sustainability assessment. A CDU focus was selected over a FMCG orientation due to its more mature developmental state. Furthermore, as identified by the GCI, the methodological considerations associated with CDU assessments are highly nuanced, influencing key decisions ranging from the selection of a functional unit to the application of system boundaries [39]. To develop a framework that meaningfully and holistically examines opportunities for purple carbon utilisation within Unilever's 'Clean Future' initiative, it is critical that these CDU specific aspects are incorporated correctly, building upon the wider academic community's existing knowledge and learnings. To this end, the review initially describes the systematic identification of pertinent standards, guidelines, and frameworks across the three assessment strands. Once collated, each independent strand is examined in isolation, a subsequent section evaluates the progress made towards their methodological harmonisation. A discussion of current strengths and weaknesses is presented, culminating in the definition of persisting gaps in terms of both knowledge and capabilities. These gaps, once known, are used to steer the development of a novel framework for the assessment of CDU within the setting of a FMCG value chain.

Chapter four examines and chronicles the development of this novel framework; combining the three assessment strands and evaluating holistic sustainability by balancing trade-offs, while simultaneously delivering easily interpreted results that help to guide movement towards achieving the 'Clean Future' initiative's goals. To support the delivery of such a research output, a guiding philosophy is initially specified, aiming to ensure that the methodology exhibits as little divergence from the ideals of the ISO standards as possible. Following this, the specific requirements of a FMCG value chain-oriented assessment methodology are explored, aiming to maximise the utility realised through application. This includes, but is not limited to, the identification of suitable data handling, decision making, and impact characterisation techniques. Multi criteria decision making (MCDM) methodologies are also evaluated and integrated to the framework. By allowing decision makers to assign importance-based weightings to each impact-indicator, a single 'overall subjective sustainability score' can be derived for each potential value chain permutation, ultimately facilitating relativistic ranking. An overall schematic of the assessment architecture is presented, detailing key methodological modules, as well as the flow of data throughout the framework. Finally, a detailed methodology for application of the framework is laid out, highlighting, and supporting key practitioner decisions.

Chapter five addresses one of the key gaps in capability recognised within the literature review (Chapter 3), tackling the development of quantified social impact pathway based characterisation models. This should be viewed in parallel to the framework development and represents what is believed to be the first attempt of its kind in published literature. As a core inhibitor to the harmonisation of assessment strands, this is a key source of value addition within the developed framework. Seven indicators are examined, covering a range of data availability scenarios, with open data from the World Bank being used to propose novel national level characterisation procedures. While limited to national level granularity and a red flag based approach, this work offers meaningful first steps towards truly holistic sustainability assessment and enables the conduction of a fully quantified assessment.

Chapter six aims to exercise and evaluate the efficacy of the knowledge developed within the previous two chapters (framework and social impact characterisation model development). The 'proof-of-concept' sustainability assessment evaluates soda ash production in the Asia and Pacific (APAC) region. As one of Unilever's largest feedstock chemicals by procurement mass, and its classification as hard to abate (with respect to GHG emissions), it is a ripe opportunity for the application of such a new and comprehensive approach to assessment. The need for this work has been highlighted by Unilever's research and development department, as well as literature searches. While a few LCA studies are present for soda ash, they are generally very opaque and, in some instances, heavily biased, as is highlighted in Section 6.3.2. It can be said with confidence that there are no holistic lifecycle assessment studies that directly and comprehensively compare different soda ash value chain permutations. Furthermore, no open literature can be found that considers the trade-offs between the environmental, economic, and social performance of soda ash production, or it's wider value chain. Therefore, the application of a triple helix-oriented approach to sustainability assessment across the cradle-to-gate value chain, building upon the scaffold laid out by McCord, *et al*. [7], constitutes a significant piece of novel and valuable research.

This soda ash oriented assessment aims to use literature data, stream tables and databases (e.g. Ecoinvent) to quantify the environmental, economic, and social impacts of a plethora of supply chain permutations. Three possible soda ash production processes are examined for their CDU potential (Solvay, Modified-Solvay, and Hou processes), with the most viable option selected for the full assessment. India is identified as the geographic focus of the assessment, owing to its position as the key soda ash market for Unilever Homecare. The value chain scenarios assessed consider a diverse range of feedstocks, energy sources and production processes. Using their respective lifecycle inventories (LCIs) as input data, the framework is scrutinised for effectiveness. Following this, the incorporated MCDM module is evaluated, example decision maker (DM) value choices are applied, and their effect on the framework's subjective recommendations examined.

The overall structure of this thesis is presented through Figure 1-5. Despite a largely linear profile, Chapters four and five can be considered in parallel due to their interdependence. A narrative bifurcation occurs at the end of the literature review, the point at which it became clear that there were two distinct areas requiring development: a FMCG specific assessment methodology, and quantified social impact characterisation models. These aspects are brought back together within the proof-of-concept study, evaluating their successes and any persisting issues in the context of APAC soda ash production. The conclusion draws on each of the three results chapters, discussing and critiquing them as a single system.

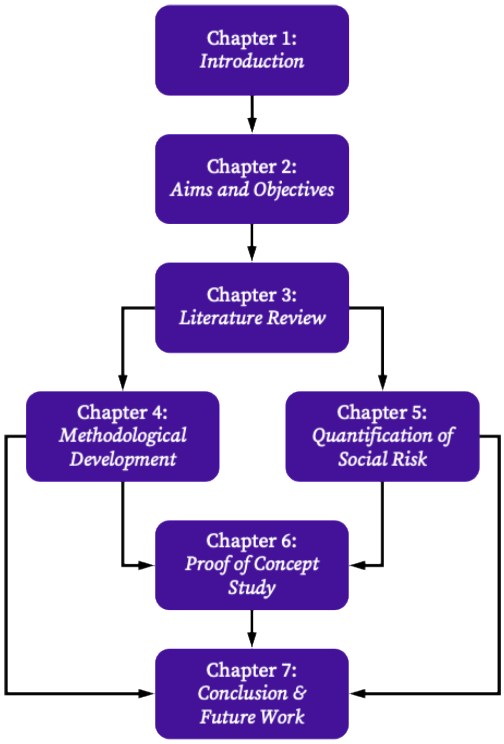


Figure 1-5 – Overview of the thesis' structure.

2 Aims & Objectives

2.1 Aims

Within many sectors of the chemical industry, sustainability issues have become key drivers within both strategic decision-making and the selection of value chain partners or suppliers. The aim of this research is the development of a novel framework, comparatively and holistically evaluating the sustainability profiles of complex chemical value chains. This shall be achieved by incorporating the environmental, economic, and social aspects of sustainability while catering to the specific utility requirements of fast-moving consumer goods (FMCG) companies. The developed framework aims to enhance strategic decision-making through integration of MCDM techniques, facilitating the inclusion of corporate decision maker's value-choices within the resulting recommendations. These goals are achieved through the systematic modularisation of existing assessment protocols, with the parallel integration of established decision-making tools. Development of the first impact pathway-based characterisation models for social assessments are also targeted, providing a basis for repeatable and transparent reporting.

Serving as a proof-of-concept based validation process, potential value chains for the production of sodium carbonate (soda ash) in the APAC region are assessed through the new framework. This study shall endeavour to incorporate only open access data for the determination of factors such as energy mixes, utility prices, and commodity chemical prices. Based upon these scenarios, a plethora of value chain permutations and feedstocks will be examined, building an assessment tool that demonstrates a tangible value addition to large scale industrial strategic decision-making.

2.2 Objectives

Chapter Objectives

- **1.0** Identify the gaps in capability within current sustainability assessment frameworks.
  - 1.1: Systematically collect relevant literature on the current state of the art for each strand of sustainability assessment (environmental, economic and social) in the context of CDU.
  - 1.2: Determine the extent to which the three strands of sustainability assessment have been harmonised and identify the current BAT for holistic assessments.
  - 1.3: Develop a taxonomic hierarchy of CDU assessment guidelines outlining the field and its progress towards meaningful strand integration.
  - 1.4: Identify the current gaps in capability with respect to holistic sustainability assessments and propose remedial strategies.
- **2.0** Develop a quantified, holistic, and value-chain oriented sustainability assessment framework redressing current gaps in capability.
  - 2.1: Specification of a guiding philosophy for framework development that is aligned with the values of the ISO 14040 and ISO 14044 standards.
  - 2.2: Identification of attributes required for the meaningful application of holistic sustainability assessment within the cont ext of a fast-moving consumer goods company.
  - 2.3: Selection and integration of an appropriate and robust multi criteria decision making technique to facilitate the ranking of available value -chains.
  - 2.4: Development of a standardised data input format, allowing for re-use of lifecycle inventory and analysis data.
  - 2.5: Development of a FMCG value chain-oriented assessment architecture capable of holistically and objectively assessing a broad range of systems while simultaneously ranking the available alternatives against decision maker value choices. .
- **3.0** Improve the repeatability of impact reporting within SIA / S-LCA.
  - 3.1: Evaluation of the current state of, need for, and feasibility of, quantified impact characterisation methods within social impact assessments.
  - 3.2: Identify suitable open-source data sets to form the backbone of a reproducible and transparent assessments inventory.
  - 3.3: Develop an initial set of quantified social impact characterisation models in which a range of data availability scenarios are covered.
  - 3.4: Apply the developed characterisation models to generate example national level results.
  - 3.5: Determine and discuss the use cases in which such an assessment technique adds value to practitioners and decision makers.
- **4.0** Conduct a 'proof of concept' study the verify the efficacy of the developed framework by assessing the production of Soda Ash in India.
  - 4.1: Identify and characterise the major incumbent soda ash production routes.
  - 4.2: Evaluate the major synthetic soda ash production processes for CDU potential and select the most promising for a full assessment.
  - 4.3: Generate a set of demonstration hub and spoke LCIs based on the selected soda ash production process to verify the efficacy of the standardised data sheet developed in Chapter 4.
  - 4.4: Demonstrate the conduction of a holistic sustainability assessment using the developed framework around the selected soda ash production process.
  - 4.5: Evaluate the effectiveness of the model's value chain selection approach and rank reversal induced by decision maker value choices.

Figure 2-1 – Research objectives.

3 Literature Review

The work within this chapter (excluding Section 3.2) has been published within Frontiers in Sustainability:

Title: The pursuit of methodological harmonization within the holistic sustainability assessment of CDU projects: A history and critical review

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Contribution Statement:

Alex Newman - Conceptualization, methodology, formal analysis, investigation, literature and data curation, writing, review and editing.

Peter Styring - Supervision and review.

3.1 Introduction

For many years, life cycle and techno-economic assessments have been seen as a vehicle through which products and processes can be compared to each other, or a relevant benchmark. Evaluating the performance of alternatives against widely accepted and quantifiable indicators provides insight into their respective performance profiles. A younger and less developed parallel sub-field [40], social impact assessment (SIA), is receiving increased attention. This has resulted in the development of its own assessment guidelines and reporting approaches. Together these aspects; environmental, economic, and social, can be considered the 'three strands' of sustainability [41]. When assessed in parallel for a given product or process, a holistic overview of their sustainability profile is obtained.

CDU technologies require these holistic assessments to manage and quantify burden shifts; occurring when improvements in one strand catalyse detrimental effects in another. A pertinent example from a parallel field is the transition to EVs for personal transport. While benefits can be seen through environmental metrics [42] [43], there is risk of producing a 'mobility underclass' through high prices and lack of access to private off-street charging facilities. Lower income households, usually commanding no off-street parking, could expect to pay £20 per' charge or 'tank' via commercial charging points; almost a threefold increase on the £7 realised by private charging [44]; a trade-off that would only be revealed through combined assessments. Such insights are extremely valuable to engineers, entrepreneurs, and policy makers alike; all of whom must collaborate to see real movement towards widespread successful CDU deployment. However, to realise these meaningful insights, holistic assessment methodologies must be identified and improved, allowing for robust integration of previously stand-alone approaches.

Despite the clear advantages of integrated holistic assessments, differences in their respective methodological approaches, or lack thereof, have historically made the three pillars difficult to align simultaneously: most notably with respect to maintaining consistent, well defined system boundaries and assumptions. This led to calls for a harmonised set of methodologies to conduct comparable assessments [45] [7] [46], providing the previously discussed holistic view of product or process performance. Outcomes from such studies have the potential to significantly improve current and future decision making, driving increased efficiency of resource allocation, particularly within R&D and policy making. When used to guide relatively fledgling fields such as CDU, this results in considerable influence over the selection of projects. Subsequently moderating progression rates towards both climate and wider sustainability goals such as the Paris Agreement [26] and UN SDGs [47].

While assessment methodologies are present for each independent strand, the research area is complex, harbouring various schools of thought. An overarching critical review of assessment methodologies and their degree of alignment is currently absent from the literature. Since 2006 multiple different standards, guidelines and frameworks have been published, targeting both generic and CDU specific applications of sustainability assessments. Movement towards the integration of strands and respective methodologies was initially slow. However, owing to increased demand for such approaches, the pace has increased in recent years. The following review examines the ongoing pursuit of this goal within CDU focused integrated assessments, identifying the progress made, common pitfalls, sources of divergence, and areas for future development. Ultimately addressing the question; “to what extent has harmonisation been achieved within holistic CDU sustainability assessment methodologies?”.

Such integrated methodologies could play a pivotal role in the validation of CDU as a climate mitigation strategy. While the field has great potential to reduce global greenhouse gas emissions, this must be robustly quantified. Integrated assessments are the best tool for this, considering not only the origin and final fate of the CO_2 incorporated within CDU products, but also the energy and resources required for its utilisation. Furthermore, they can provide a direct comparison of CDU processes against the current industry standard, verifying better performance over a wide range of available impact categories, including economic and societal aspects.
CDU technologies are usually highly energy intensive. The green generation of this energy must be traced and accounted for to confirm any sustainability improvements; alternate fossil-based energy mixes result in highly ambiguous, and sometimes non-existent, emissions savings. Furthermore, issues around infrastructure (e.g. pipelines, engine fuel specification, etc.) and process operating costs have historically plagued the economic viability of CDU projects. The associated transition phase and elevated consumer prices go on to catalyse detrimental societal effects, as seen in the EV example previously. Understanding and combatting these interlinked sustainability issues will enable faster and more effective development within the field.

3.2 Aims and Objectives

Table 3-1 - Objectives for Chapter 3.

Objective	Specification
1.1	Systematically collect relevant literature on the current state of the art for each strand of sustainability assessment (environmental, economic and social) in the context of CDU.
1.2	Determine the extent to which the three strands of sustainability assessment have been harmonised and identify the current BAT for holistic assessments.
1.3	Develop a taxonomic hierarchy of CDU assessment guidelines outlining the field and its progress towards meaningful strand integration.
1.4	Identify the current gaps in capability with respect to holistic sustainability assessments and propose remedial strategies.

3.3 Methodology

Guidance around the conduction of sustainability assessments is broad, encompassing a diverse range of methodologies. This review aims to collate and assess only CDU specific guidance documents, or those from which these are derived. Their assessment is meaningful due to sustainability assessment’s importance as a guidance tool in the development and roll out of CDU technologies. Secondly, to ratify that both the diversity of needs, and nature of methodological hurdles, exhibited by different sectors necessitates a departure from generalised guidance. The identified approaches are reviewed, identifying areas in which harmonisation is achieved, and those where it is still lacking.

3.3.1 Identifying Literature

A semi-systematic approach (Figure 3-1) was taken to the collation of literature within this review. Initial searches were conducted using bibliographic databases and academic search engines; primarily web of science, google scholar and science direct. Together these provide access to a vast majority of academic literature. Search terms initially focused on the individual assessment strands, identifying cornerstone guidelines. Common identifiers for the respective strands (e.g. LCA, E-LCA, life cycle assessment, etc.) were utilised, coupled with “standards”, “guidelines” and “framework”. This revealed the major guidance documents, later confirmed by their widespread proliferation within consulted assessments and inter-guideline cross-referencing.

Secondary literature was collated in the form of existing reviews, focusing on individual assessment strands. These are to determine the overall ‘topography’ and development of the respective research areas. Additionally, these serve to provide large numbers of relevant pre-screened primary sources. Where possible, multiple secondary sources were consulted within the same strand, aiming to identify and prevent any potential propagation of bias.

A second round of literature identification was conducted, this time sequentially adding the terms CCU, CDU and CDUS to fielded searches. The purpose of which was to identify any sector specific guidance documents or assessments. In some cases, this returned highly relevant documents, such as the GCI (Global CO_2 Initiative) guidelines. Other times, no relevant publications were identified. In these lacking cases, it will be assumed that no specific guidance is available beyond the previously collated general guidelines. A third and final search of literature was carried out, including the terms ‘holistic’, ‘harmonised’, and ‘integrated’. This was by far the least lucrative round of literature searching, attributable to the infancy of integration efforts.

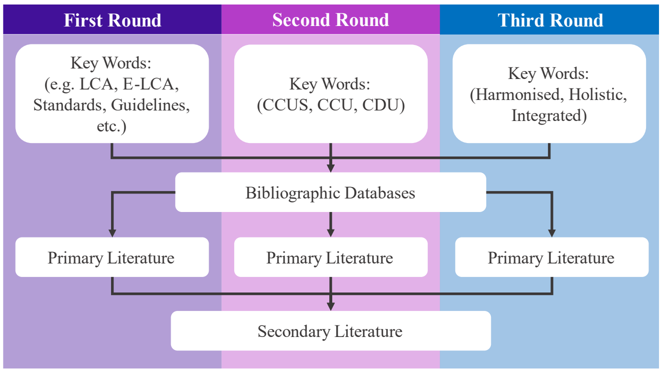

Figure 3-1 - Schematic of the semi-systematic literature search employed

3.3.2 Approach to Analysis

A review of harmonisation and integration within CDU focussed sustainability assessment is novel within literature. Consequently, this work aims to evaluate the current best practices and most promising methodologies. While this requires an initially broad and general approach to methodological comparisons, it is hoped that a strong foundational understanding of the field and its current shortcomings and successes are contributed. Subsequent reviews around the specific issues identified herein would further enrich understanding and support continued improvement of assessment techniques.

Initially, relevant frameworks and guidelines pertaining to each independent strand are dissected. Examining the structures and principles of the methodologies facilitates the construction of a ‘taxonomy’ of guidance, charting the development path towards a holistic approach. Integrated approaches are reviewed, identifying any loss of resolution or conflicting schools of thought. Comparability, clarity of results communication, robustness and transparency within each methodology will be considered the metrics for success.

Beyond these largely intangible aspects of the methodologies, the approaches to indicator calculation will be examined and comparisons drawn between strands for both independent and integrated approaches. The standardisation of both procedures and assessment structure are deemed a core aspect of harmonisation. Consequently, the LCA strand will be viewed as the template for methodological homologation, owing to its position as the most broadly utilised and mature technique within sustainability assessment. Constituent components within the goal and scope of each assessment strand are tabulated for cross comparison. As critical parts of initial assessment development and definition, this provides new insights into the levels of integration attainable and any residual sources of methodological conflict for future resolution.

3.4 Review of Literature

To evaluate the state of holistic harmonisation within sustainability assessment, the three constituent strands are initially examined independently. Each initially emerged as standalone assessment methodologies, yielding the single-faceted approaches found through the literature search. Most of these single stranded assessments focus on general application; however, some have been refined and iterated, producing CDU specific approaches. Guiding principles and key methodologies for each are laid out in the following sections, detailing the foundations upon which later integration efforts rest.

This subsequent examination of the shift towards integration focuses on the harmonisation methodologies presented in literature, considering their success or failure in handling and homologating methodological hurdles. Notable areas include assessment structure, boundary alignment, indicator selection and calculation, scenario generation, and handling of assumptions. Common errors seen within the assessment of CDU projects will also be examined; reviewing the effectiveness of mitigation strategies provided by sector specific guidelines.

Assessments focusing on CDU projects necessitate methodological decision making support that is overlooked in general frameworks. For example, a benchmark system must be assessed, a consequence of the disruptive nature of CDU technologies. Further complications arise from the broad range of TRLs observed in CDU, generally spanning levels 3-8, stemming from issues around data availability and inter-assessment comparability.

3.4.1 Lifecycle Assessment

Environmental assessments of products predate the use of the term LCA, appearing within literature in one form or another since the 1960’s [18]. Since then, large strides have been made; initially aiming to better define the field, latterly seeking a standardised, robust, and reproducible approach. The 1960s and 1970s see the conception of what would become modern LCA in response to increased public concerns around energy use, resource efficiency and pollution [48]. These studies initially focused solely on energy flows [49] [50] [51]. System based approaches to assessment, similar to those now used, emerged in 1974 with a US EPA study on alternative beverage containers [52]; although this methodology was not initially adopted broadly. The 1980s and 1990s exhibit significant methodological divergence, while failing to cultivate meaningful scientific discussion [18]. This ultimately prevented a single methodology from gaining wide acceptance as an assessment tool, primarily due to comparability issues between studies.

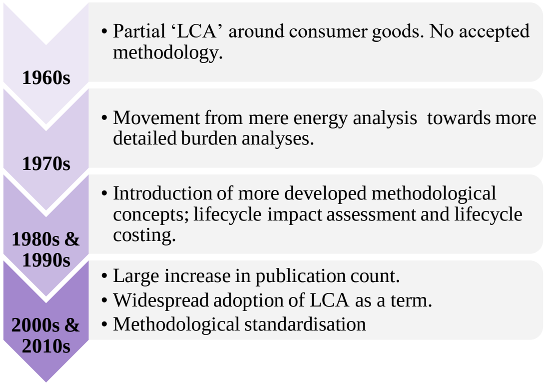

Figure 3-2 - Brief outline of LCA's methodological history

Publications including the term 'LCA' begin to appear in the late 1990s. Standardisation was sought in this period, leading to the convergence of environmental impact studies under this unified umbrella. The number of published articles citing 'life cycle assessment' as a key word can be seen in Figure 3-3. Publication data obtained through literature search demonstrates the increase in application over the early 21st century, exhibiting rapid growth of the field after 2005. Studies from 1960-1995 do not appear as the term LCA had not yet been coined.

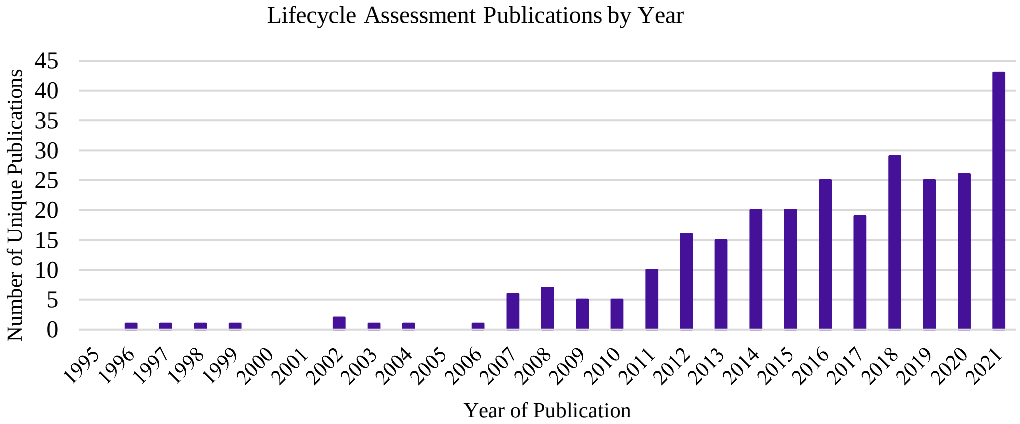

Figure 3-3 - Distribution of LCA publications by year. Data collected using Web of Science, using filters of; author keywords of 'lifecycle assessment' and year published of '1960-2021'.

LCA in its modern form accounts for the environmental impacts of a product or service throughout its entire life cycle, spanning from cradle to grave, i.e., from raw material extraction through to final disposal. At each stage, the product system interacts with the environment, consuming natural resources and emitting pollutants. Assessments aim to quantitively assesses these interactions and their potential environmental impacts [53]. Correct application delivers [54]:

1. A breakdown of environmental loads to constituent unit operations or life cycle stages; identifying areas for optimisation.
2. Internal comparisons of products or processes.

3.4.1.1 ISO Standards

In 2006, ISO 14040, and the broader ISO 14K series, became the first internationally recognised and standardised methodological framework for LCA. Importantly for topic of this paper, the ISO technical committee recognised the need for parallel techniques assessing economic and societal impacts, an early call for holism. ISO's key achievement was the crystallisation of fundamental principles for LCA. These have subsequently been adopted by all significant guidelines and include [55];

- *A life cycle perspective*, considering all operations from raw material extraction to end of life treatment or disposal.
- *Environmental focus*, recognising the exclusion of economic and social factors from the scope of an LCA; suggesting the implementation of parallel assessments for more extensive studies.
- *Relative approach and functional unit*, analysis and results based on a quantifiable attribute of the product (e.g. mass, energy content, or function).
- *Iterative approach*, in which data is refined or revisited based on quality requirements implemented within subsequent stages.
- *Transparency* of execution and interpretation.
- *Comprehensiveness*, including all system attributes pertaining to natural environments, human health, and resource use.
- *Priority of scientific approach*; basing methodological decisions on natural science. Resorting to social and economic sciences only when necessary.

ISO present a four-phase methodological approach (Shown in Figure 3-4), subsequently adopted as a mainstay within broader sustainability assessment methodologies. The respective components of this general methodological framework are subject to more detailed examination within ISO 14044 [56], an accompanying standard. This second document prescribes specific methodological requirements and guidance for the correct execution of studies. Many previously divergent aspects within assessments were standardised, reducing inconsistencies around methodological structure and practitioner choices. This aimed to eliminate comparability issues that had previously barred LCA from acceptance as an assessment tool.

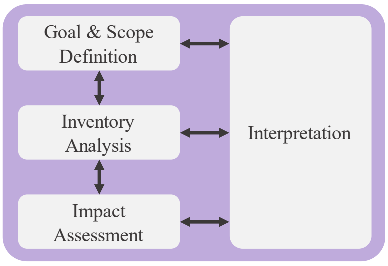

Figure 3-4 - Standardised assessment phases for LCA as developed within ISO 14040 [55]

Introduction of impact quantification in terms of a functional unit ensures that results are presented in a comparable format based on product functionality. Practitioner guidance around cut-off criteria is also developed, systematically handling gaps in assessment coverage, ensuring results are representative of the real world. While the methodological steps for this procedure are detailed, they lack quantification. Instead relying on the practitioner's good judgement, generating a novel source of study misalignment and comparability issues.

Multiproduct systems represent a historically persistent challenge within LCA. Questioning how burdens should be apportioned within such systems where more than one saleable product is generated. ISO approaches standardisation around the issue pragmatically, introducing a hierarchy of handling methods. These are, from most to least preferable; avoidance, physical relationship (e.g. mass), or other relationship (e.g. economic value) [55]. A one size fits all approach is not feasible for allocation, owing to the differing aims of studies and application of products. Recognition of such complex methodological considerations proves to be ISO 14040's strength.

Data collection is widely recognised as a complex and resource intensive procedure in LCA. Helping to navigate this, ISO14044 provides collection sheets for use by practitioners [56]. This assists with the organisation of data around given unit operations or life cycle stages, generating inventories for system inputs, outputs, transport distances, etc. Additional benefits are realised through this systematic data handling, most notably improved transparency. Data quality reporting is also scrutinised, requiring improvement where quality is insufficient (or where data is missing); reflecting the iterative approach laid out by the guiding principles. ISO assess quality in terms of ten factors: temporal coverage, geographical coverage, technology coverage, precision, completeness, representativeness, consistency, reproducibility, source, and uncertainty [56]. This approach invites the use of pedigree matrices to track validity across the factors, resulting in a robust and documented assessment of data quality.

Overall, ISOs 14K series likely constitutes the largest single leap forward in LCA methodology. It delivers broadly applicable and standardised approaches to structure, methodological hurdles (allocation, cut-off criteria, etc.), and fair comparative assessments. However, several key decisions remain at the discretion of practitioners, potentially affecting the integrity of the results and insights generated. Key examples include selection of indicators and characterisation methods, formulation of assumptions, and derivation of system boundaries. In attempts to mitigate these factors many offspring guidelines and frameworks have been developed upon the foundations laid down by ISO 14K.

3.4.1.2 ISO Derived Guidelines

Chronologically, the first significant ISO derived guidance is the International Reference Life Cycle Data System (ILCD) Handbook (2010) [21]. Requested by the European Commission, the objective of the handbook was to inform the development of subsequent sector specific assessment guidelines, applying current best practices and facilitating more comparable studies. The outcome is consistent, robust, and quality-assured frameworks for assessments of similar products on an equivalent basis, validating ecolabelling claims. Resulting off-spring frameworks are ISO compliant, with the handbook acting as a more granular extension of ISO14044. Structured around Shall/Should/May guidance, the document lays out both required and recommended methodological steps, clarifying procedure for practitioners.

The ILCD Handbook makes progress through the narrowing of methodological choices left to the practitioner via bolstered guidance, reducing subjective influences on results. Two veins of assessment are addressed specifically: decision making (micro, meso, and macro) and accounting. Despite making progress, the handbook fails to tackle some legacy issues within LCA. Quantified rules around cut-off criteria are not developed in any meaningful way, only the reporting of targets (e.g. % reporting completeness) and omissions. Furthermore, the approach to selection of impact indicators is not developed. While these shortcomings are symptomatic of the handbook's broad objective, it prevents the comprehensive closure of many methodological gaps seen within the preceding ISO standards.

As a successor to the ILCD handbook, the European Commission instructed the development of ISO compliant 'Product Environmental Footprint (PEF) Category Rules' [57]; reacting to regular calls for rules around specific product categories [58] [59] [60]. The delivered rulesets develop upon the guidance provided in the ILCD Handbook, generating product specific LCA guidance through pilot schemes. PEF targets enhanced harmonisation within product categories; they provide detailed instructions for goal and scope definition, system modelling requirements, and standardised impact assessment categories and characterisation approaches [61]. While mandated impact indicators are desirable for comparability, they significantly reduce methodological applicability; primarily through a reduction in assessable goals and scopes. Despite this, the tightening of methodological procedure delivers notable benefits, such as an aggregated indicator score. However, for harmonised CDU applications, the PEF category rules' rigidity make them challenging to align with economic and social strands. The most likely origins for these issues are data collection and inventory structure. Consequently, the PEF Category Rules are not recommended for use in assessments targeting strand integration. Furthermore, the specification of guidance based on the product means that CDU relevant impact indicators and methodological decisions may be neglected; a consequence of the guidelines needing to accommodate competing, non-CDU, production routes.

The final standalone LCA guidance identified is the GCI's 'LCA Guidelines for CO_2 Utilisation' [62]. First published in 2018, a revised version was presented in 2022 [23]. With LCA's general methodology having been developed significantly in the preceding decade, CDU specific guidance remained lacking. This impaired comparability through practitioners' divergent methodological decisions around factors including system boundaries and functional unit selection. GCI used the ISO standards [55] [56], ILCD Handbook [21] [63], chemical engineering textbooks [64] [65] [66] [67] and other literature sources [68] [69] as their foundation. Again, following the Shall/Should/May format for guidance application, requirements of the ISO standards are adhered to fully. However, specific areas critical to CDU technologies and their deployment are necessarily more methodologically constrained. These include the selection of CO_2 source, system boundaries, functional unit selection, and assumptions around utility sources.

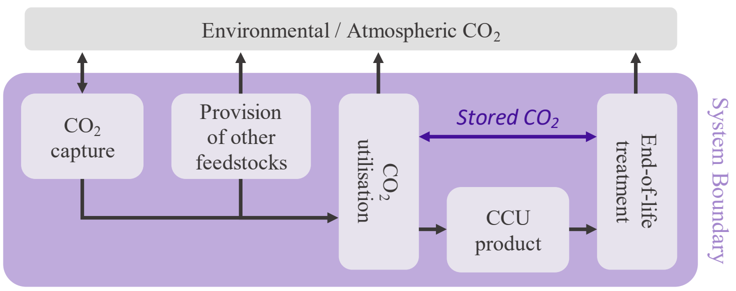

Figure 3-5 - Generic example of correct system boundary for a cradle to grave CDU LCA. Adapted from the Global CO_2 Initiative [69]. 'Provision of other feedstocks' includes the generation of electricity and other utilities.

CDU LCA results are highly sensitive to differences in system boundary, notably CO_2 sourcing. GCI therefore require that the energy requirement and carbon intensity of CO_2 capture must be included; tackling the commonly observed pitfall of treating anthropogenically captured CO_2 as a negative emission without its associated burdens (that is, for every kg fed; $GW_{CO_2-Eq.} = -1\left(\frac{kg_{CO_2}}{kg_{CO_2-Eq.}}\right)$) [23]. Thus, any post-capture purification, compression, and transportation must be quantified and assessed. Standardisation in this area delivers more comparable studies and legitimate impact quantification. An example GCI compliant system boundary for the correct inclusion of CO_2 capture is detailed in Figure 3-5.

Often, the assumptions made around utility provision in CDU assessments are regularly overly optimistic or infeasible. These range from excess green electricity generation to unrealistic grid capacity and resilience scenarios. When examining electricity supply, GCI give a hierarchy of options for assessing environmental burden; ideally utilising real world (geographically specific) data, followed by representative grid mix, and finally net-zero [23].

Also targeted by GCI is the misalignment of functional unit selection in precursing literature. The result is a flow diagram (Figure 3-6), prescribing the appropriate functional unit [62]. A unified approach is achieved, ensuring that products with the same intended application are assessed on an equivalent basis, while also accommodating the broad range of CDU technologies and products. This advancement demonstrates the need for GCI's work on CDU guidelines; disseminating tools for sector standardisation that are not possible at a more generalised level due to differing methodological requirements.

Examination of the impact assessment approach put forward in the GCI's methodology also reveals movement towards standardisation. While a specific set of impact indicators is not mandated, it is suggested that European studies employ those curated by the JRC (European Commission's Joint Research Centre) [23]. However, after indicators are selected, GCI require that CML (Institute of Environmental Science, University of Leiden) [70] characterisation models are employed. While impact indicators must be left at the practitioner's discretion to allow for varied assessment goals and scopes, standardisation of characterisation models greatly aids comparability between assessments.

Overall, GCI meaningfully enhance guidance for the application of an ISO compliant LCA methodology within CDU. Major hurdles around practitioner choices have been removed, with steps taken to harmonise goal and scope setting between assessments of comparable products (e.g. functional unit selection and system boundary definition). The result is a strong environmental assessment strand, offering robustness and repeatability. Future work in the area may benefit from the partial standardisation of impact indicator selection; potentially with assessment specific additions made at the practitioner's discretion to accommodate broader goals and scopes. Further guidance around allocation procedures would augment assessments, especially given the tendency of CDU processes to generate multiple products; currently the ISO methodological hierarchy is adopted without further development. However, care should be taken to ensure that allocation method selection does not encroach on the range of possible goals and scopes.

Beyond these examined methodologies, the National Energy Technology Laboratory (NETL) provide a US based framework for CDU specific LCA [71], developed in parallel to GCI's. However, due to the geographical specificity of the work it self-eliminates from broader standardisation efforts. For this reason, it is not discussed further in this review, despite utility in North America.

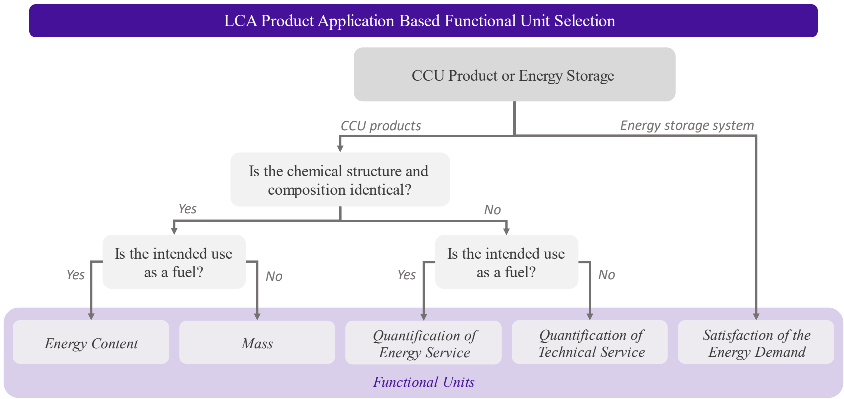

Figure 3-6 – Flow diagram for the identification of the selection of an appropriate functional unit within CDU oriented LCAs. Adapted from the Global CO_2 Initiative [62].

3.4.1.3 Current State of LCA in CDU

To summarise the current state of LCA guidance, the field has reached a high degree of both maturity and holism. The ISO standards provided a broad but robust foundation for steady development, pioneering many procedural steps that see adoption in subsequent more specialised CDU guidance. Although some approaches' rigidity complicates harmonisation (notably the PEF Category Rules), a clear path to CDU specific assessment can be identified (see Figure 3-9). The development of LCA can, in many ways, be seen as a cascading set of guidance documents; these hail from the ISO standards and incrementally grow more specific in nature. When pursuing a holistic and harmonised methodology, a trade-off must be managed between flexibility, in the interest of strand alignment, and rigidity to aid comparability.

Comparability has been enhanced through incremental refinements, significantly reducing the 'apples vs oranges' [45] problem. Furthermore, all current methodologies found in literature utilise a BFD (block flow diagram) approach towards system modelling [55] [21] [53] [57] [27] [62]. This identifies consequences, or impacts, of resulting environmental interactions via evaluation of material and energy flows crossing the system boundary (elementary flows). The functional units used, and therefore the basis of assessment results, are also standardised through GCI guidance. Impact characterisation is universally achieved through the application of published approaches. However, despite the specified use of CML models, the selection of indicators assessed are not yet standardised; identified earlier as a potential area for tentative guidance development.

Beyond this, the application of cut-off criteria is handled non-uniformly, with guidelines failing to detail specified thresholds. This is unlikely to be resolved through future iteration of the guidelines. Their rigid specification would ensure that resulting frameworks are incompatible with many assessment goals and scopes, as exemplified by the PEF Category Rules. In essence, a one size fits all methodology would be inherently flawed.

The presence of life cycle databases such as Ecoinvent greatly supports practitioners, with over 18,000 inventory datasets [72]. However, emergence of such tools necessitates methodological maturity in order provide utility, enabling the standardisation of information formats and underpinning calculations. Three primary benefits can be observed as a consequence of its use: practitioner workload reduction, greater impact pathway transparency, and the use of common data inputs between assessments. Without Ecoinvent, LCAs would require significantly longer to complete and exhibit a much lesser degree of comparability.

3.4.2 Technoeconomic Assessment

TEA evaluates the economic demands of research, development, demonstration, and deployment of technologies [22] [73]; quantifying the production costs and size of market. Approaches have historically exhibited non-standardised approaches, a symptom stemming from the lack of widely accepted guidelines [27] [28], general or otherwise. In fact, it has been identified within literature that CDU is an area ripe for TEA standardisation [74], seeking an answer to the continued 'apples vs oranges' comparability issue [45]. Furthermore, augmented policy development, decision making, and R&D funding allocation may be realised with such an assessment tool [73]. This lack of a standardised approach has not hindered the rate of TEA publication, demonstrating the assessments utility, even in non-standard form. Figure 3-7 shows the yearly number of TEAs observed in literature. Within this data a clear upwards trend is observed, publication count increases year on year without exception.

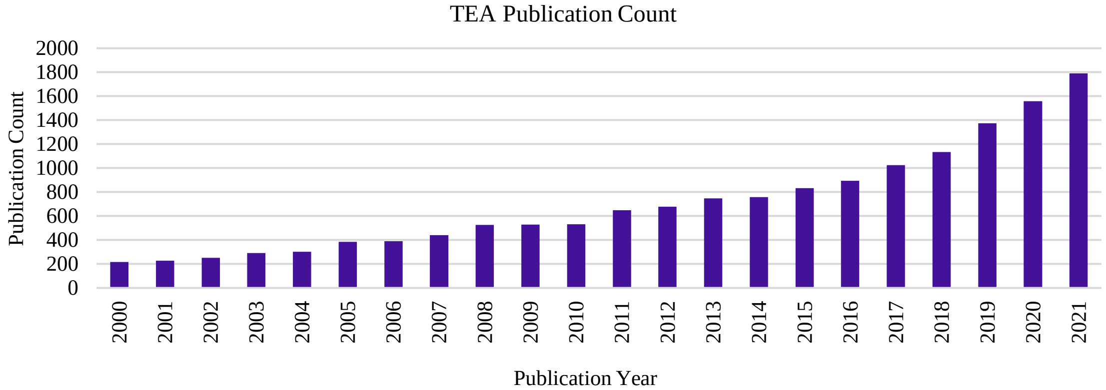

Figure 3-7 - Distribution of TEA publications by year. Data collected using Web of Science, using filters of; author keywords of 'technoeconomic assessment', 'techno-economic assessment' and year published of '2000-2021'

Assessments are not limited to one life cycle phase, many extend to include the upstream and downstream operations, although the production phase is typically the focus. LCC (life cycle costing) has historically been used for this on a cradle to grave basis [75] [76] [77]; with studies carried out around its potential integration to LCA [78] [75] [79]. LCC typically exhibits a cost driven focus, regularly neglecting technical and profit-based indicators [27], inhibiting its application within a decision-making and development context. By instead utilising TEA, increased scope flexibility aids potential integration with LCA. This wider approach to assessment of economic sustainability facilitates the identification of economic drivers throughout complex value chains, offering significant applicability within both CDU projects and technology development.

Zimmermann *et al.* identify that TEA assessments of CDU projects did not, at that point (2017), follow a common approach [45]; this included analysis of both government reports and academic papers. The finding was later ratified by the GCI, identifying two CDU-relevant methodologies [80] [81]. However, after analysis, both were deemed too generic for direct application to CDU cases. Approaches seen in previous literature are broadly limited to those presented in chemical engineering textbooks [27]; primarily Peters *et al*. (2003) [82], Sinnott and Towler (2009) [83], and Turton *et al*. (2012) [84]. Inevitably, utilisation of varied approaches prevents meaningful comparisons between studies of similar systems. The application of generalised guidance encounters similar issues to those seen within LCA, divergence in methodological application and assumptions, necessitating both standardisation and transparency. Typical pitfalls associated with CDU TEAs are identified; including but not limited to [27]:

- Alignment with LCA methodologies
- System boundaries
- Indicator selection
- Lack of TRL assessment
- Characterisation model application
- Derivation of CO_2 prices

3.4.2.1 GCI Guidelines

In 2018, the GCI released standalone CDU specific TEA guidance [22], developed in parallel with their LCA counterpart. These were produced in co-operation with around 50 international experts and informed by a systematic literature review incorporating contemporary best practices within industry, academia, and policy. The resulting ‘first of a kind’ approach is purposefully harmonised with LCA, taking structural inspiration from the ISO standards [55] [56], and ILCD Handbook [21]. In addition to these structural developments, GCI deliver practitioner guidance around assessment areas that exhibit high sensitivity within CDU applications. In addition, they call for the development of a new ISO standards for TEA. This would be parallel to the ISO 14K series, potentially ratifying GCI’s methodological approach [27]. The following section will outline CDU specific guidance from only the GCI work, owing to lack of alternative guidelines.

GCI systematically tackle the common CDU TEA pitfalls identified by Zimmermann, *et al.* through the provision of additional methodological requirements and guidance. The same four phase structure is adopted as seen in LCA (see Figure 3-4), laying the groundwork for harmonisation. This is supported by the original ISO 14040 standards recognition of the need for parallel assessment methodologies [55]. Analysis on the basis of a functional unit is also adopted, selected following the same flow diagram seen for CDU LCAs (see Figure 3-6). Contrary to prior TEA approaches, requirements are laid out for both the goal and scope definition, carrying benefits for both practitioners and comparability [27].

Allocation, for multi-product systems, is handled in harmony with the LCA guidelines. ISO’s methodological preference hierarchy is adopted; however, with additional scope for practitioners to “follow any principle that ensures meaningful results” [27] when the goal or scope requires. This significantly reduces the lack of both standardisation and harmonisation previously seen around allocation in both general and CDU specific TEA. Given the financial orientation of the strand, it is perceivably of benefit to consider allocation through economic value when conducting stand-alone assessments.

Augmented guidance around the definition of system boundaries results in a significant reduction in the scope of practitioner decisions. However, in contrast to the LCA guidelines, there is a provision for the application of gate-to-gate boundaries. Consequently, R&D, or corporate perspective studies can assess over a single value actors’ section of a supply chain, broadening applicability. Capability for cradle-to-gate and cradle to grave assessments is not impacted, safeguarding subsequent assessment strand harmonisation and integration.

GCI refine practitioner support around product systems where carbon capture is employed, a target of the guidelines, defining boundaries using information provided within ISO 27912 [85] and ISO 27919 [86] [87], the standards for carbon dioxide capture; a significant step towards easily comparable assessments. The procedure prescribed for the evaluation of CO_2 source is based upon that of the counterpart LCA guidance, this time also accounting for the price of capture. Two levels of granularity are presented for the assessment of capture; selection is based largely on the goal and scope of the assessment. Most preferable is the assessment of a specific capture process and supplier, using primary data. Alternatively, where this is not feasible, an industry or technology average value (secondary data) can be used for technical and economic data points.

The nature of TEA requires data specificity both geographically and temporally; these factors influence employed assumptions and sources of input data. Consequently, guidance is developed to aid practitioners while navigating these aspects of assessment. As with GCI's parallel LCA guidelines, geographical and temporal considerations introduce nuances around the assessment of process inputs, outputs, utilities, and scenario modelling.

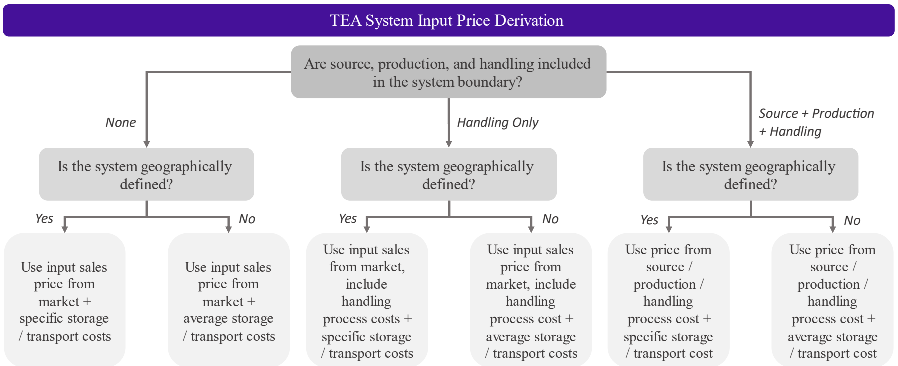

Figure 3-8 - Derivation of commodity input prices as a function of system boundaries. Adapted from the Global CO_2 Initiative [27]

Identified as a common source of error within assessments [27], derivation of feedstock prices (detailed by Figure 3-8) and sources are critical to study validity; perhaps the most obvious example within CDU projects is CO_2. Prices seen in literature can vary widely. Costs between 5 USD – 180 USD per tonne CO_2 are reported (although a small number of sectors exceed this) [88] [89] [90]. With large quantities used within CDU, importance of correct estimation on an assessment specific basis is clear. Clarification of the required concentrations and purification steps is crucial, facilitating selection of a suitable supply and relevant cost estimates. GCI mandate that the lowest concentration source technically feasible should be used (not simply that with the lowest price), while ensuring compatibility with the coupled process(es). This requirement demonstrates the guidelines specialisation around CDU. Utilisation of the lowest possible grade of CO_2 preserves purer sources for other CDU deployments that require them. Furthermore, where the capture is within the system boundary, relevant CapEx, OpEx, purification, compression, and transport costs should be included when estimating CO_2 price [27]. Where capture is excluded from the system boundary, literature should be used to estimate cost. Average prices should be obtained by consulting reports detailing specific capture technologies or sources; GCI detail multiple useful governmental and organisational data sources. Provisions are made for studies with varied geographic specificity, suggesting the use of prices at the highest degree of spatial accuracy available. Typical pitfalls around CO_2 costing identified in literature include [27]:

1. Assumption of zero cost.
2. Assuming ETS (emissions trading scheme) price or emissions tax as the full procurement cost.
3. Use of GHG (greenhouse gas) abatement cost as a proxy for capture cost.

Such pellucid methodological guidance around a highly sensitive variable in CDU's economic performance significantly aids comparability. Furthermore, it safeguards assessments from the assumption of overly optimistic scenarios, results, and conclusions.

The GCI recognise the importance of assessment scenario development within TEA. Large amounts of practitioner guidance are provided relative to that seen in LCAs (typically less sensitive to market, spatial and temporal factors, excluding grid mixes). Measures extend to requiring the adoption of a H_2 production method that has reached a TRL of 9, indicating a mature and viable route (such production methods can be identified within Ullmann's Encyclopaedia of Industrial Chemistry [91] and HIS Markit's Chemical Economics Handbook [92]). This ensures that overly optimistic scenarios are not used to make the assessed system appear more favourable across the selected indicators. The primary benefit seen through this bolstered guidance and methodological constriction is the mitigation of typical practitioner pitfalls surrounding the assessment of hydrogen pricing seen within previous TEAs [27]:

1. Assuming all low TRL production routes will reach technological maturity.
2. Economically favourable yet environmentally burdensome production (negating the proposed benefits of CDU)
3. Basing production on the utilisation of intermittent electricity inputs. Omitting associated trade-offs such as repeated start-up and shutdown mechanisms, CapEx, and OpEx.

Pricing of electricity, a significant input to many CDU processes, is also examined. It is determined that full production costs should be evaluated, eliminating a previously major source of system boundary divergence in TEAs of the sector. If necessarily excluded from the system boundary, GCI state that market data must be used to avoid the assumption of a zero-input price (as seen in some TEA studies) [27]. The guidelines present several literature sources for electricity pricing: Eurostat's energy database [93] for European cases, and EIA (Energy Information Administration) database [94] for North America. CDU TEAs for low TRL processes have previously made assumptions of zero or negative electricity prices, complicating literature comparisons. Furthermore, GCI identify that changes in relevant input markets should be accounted for (e.g. commodity prices, competing technology or regulatory differences); a practice not seen within the counterpart LCA guidelines. Returning to the previous example of CO_2 procurement, prices are relatively uncertain as a result of these market forces, representing a common source of errors in literature assessments.

Within precursing CDU TEAs, indicator selection is far from standardised, often with multiple alternatives used for the same criterion [45]. GCI identify TRL, OpEx (operational expenditure), and CapEx (capital expenditure) as frequently employed indicators. However, the guidelines note that their definitions and characterisation methods differ greatly [27]. This is rectified within the developed TEA guidelines through provision of standardised definitions and calculation approaches. For both OpEx and CapEx calculations, differing approaches are suggested based on process TRLs, accounting for respective differences in data availability and uncertainty.

If the goal and scope target more specific insights, additional indicators can be appended at the practitioners discretion utilising previously noted textbooks [82] [83] [84], delivering valuable assessment flexibility.

3.4.2.2 Current State of TEA in CDU

In spite of reliance on a single guidance document, notable progress has been made around CDU oriented TEAs. The GCI's guidelines represent the first attempt at sector specific guidelines, strengthening many of the weakest methodological links. Making use of the ISO standards as a template, the developed guidance is successfully harmonised with LCA, realising the benefits of transparency and an iterative approach. Major assessment stages are therefore congruent with the counterpart LCA methodology, facilitating integrated studies. Key aspects of application to CDU are addressed, primarily through enhanced practitioner guidance around the setting of CO_2 sources system boundaries, generation of assessment scenarios, and the estimation of key input prices. These highly sensitive factors in the economics of CDU had not previously been assessed robustly in existing literature. Compounding this, the suggestion of data sources for sensitive inputs should further improve homologation between studies. While data sources are available, TEA would significantly benefit from practitioner friendly databases comparable to Ecoinvent within LCA, providing support for the derivation of input and utility prices.

Despite this progress, the non-uniformity of impact indicators assessed still threatens inter-assessment comparability. However, the prescription of functional units as well as characterisation models for commonly utilised indicators will partially alleviate this issue; effectively 'shepherding' practitioners into using the same approach. Additionally, GCI do not list policy makers as a stakeholder group within the guidance document, a divergence from LCA. This may prove to be a limitation given the criticality of policy decisions on the development of emerging CDU technologies.

3.4.3 Social Impact Assessment

The third and final assessment strand examined in isolation is SIA (also commonly referred to as S-LCA). As the youngest and least standardised of the 'strands', social assessments represent an area of growing interest and relevance [30] [31] [32]. SIA primarily focusses on corporate social responsibility, and can be defined as; "the process of identifying the future consequences of current or proposed actions, which are related to individuals, organisations and social macro-systems" [7] [95]. Vanclay, 2003, proposes that any developed guidelines should be derived from core values and principles [96] such as the UN SDGs [41]. When considering comparability of assessments, Pollok *et al*. notes that while the ISO format is generally accepted within social assessment, it is not implemented rigorously; often resulting in major divergences [30] and complicating the harmonisation and subsequent integration of assessment strands.

Historically, the integration of social factors within engineering assessments has been recognised as challenging. The development of SIA methodologies is chronicled in a review by Huarachi *et al*. [29], defining four distinct phases (Summarised in Table 3-2). The final phase, fittingly for this review, is 'the search for standardisation'. Beginning in 2017, the endeavour is ongoing, tackling the methodological divergence exhibited within 'the development years'. Despite this continued lack of standardisation, the 2010s saw the emergence of SIA into the mainstream of sustainability assessment.

Table 3-2 – Developmental stages of S-LCA or SIA and their associated points of notable progress. Adapted from Huarachi et al. [29]

Phase	Year	Notable Progress
First steps towards S-LCA	1996-2009	• O'Brien eat al. (1996). The first and only assessment of societal impacts from a lifecycle perspective conducted in the 1990s. Producing a methodology termed Social and Environmental LCA (SE-LCA). • From 2006 articles relevant to the field were published every year. Although these were reviews, lacking further methodological development.
The uncertainty years	2009-2012	• UNEP/SETAC S-LCA guidelines published, mirroring the ISO 14040 structure. Currently the largest step towards a broadly accepted methodology. • Databases for collation of information regarding S-LCA begin to appear. • 2010-2012 sees a latency period between development of a theoretical basis and tangible practical applications.
The development years	2013-2016	• 2013 sees a large increase of S-LCA based publications, totalling 20. Partially attributed to the release of UNEP / SETACs methodological sheets, aiding practitioners. • Suggestion of MCDA integration within a S-LCA context. • UNEP / SETAC remain the dominant guidelines, others are still proposed. • Further development of databases. Pertinent examples being the Product Social Impact Lifecycle Assessment (PSI-LCA) and Social Hotspots Database (SHDB). • Proposal of quantification methods for qualitative social impacts. • Emergence of many methodologies and approaches to the assessment strand
The search for standardisation	2017-Ongoing	• S-LCA achieves recognition as a valuable tool in the assessment of sustainability. • Number of methodological proposals without application decline significantly. • UNEP / SETACs guidelines remain the most broadly applied. • Discussion begins around the handling of positive impacts and their inclusion. • SHDB achieves widespread use within generic S-LCAs

While many publications have evaluated the social acceptance of CDU, a majority reporting favourable community perceptions [97] [98] [99] [100] [101], the need for an impact assessment is highlighted in multiple works [45] [30]. Zimmermann *et al*. identify a general absence of SIA assessments within low TRL technologies [45] [102]. This gap in literature must be closed if meaningful SIAs are to be achieved around CO_2 utilisation. As of writing, no standalone CDU specific SIA methodology has been proposed; with one framework for integrated LCA/TEA/SIA developed by McCord *et al*. [7].Despite this, some sector orientated approaches have been discussed in literature for other fields, validating the concept; examples include minerals [103] and mining [104].

3.4.3.1 Methodological Approaches

Social impacts are most commonly reported relative to the UN SDGs (Sustainable Development Goals) [47] or GRI (Global Reporting Initiative) [35] [7] [105]. However, these are typically carried out around deployed operations rather than during R&D [7] [45], a problematic characteristic considering the low TRL nature of many CDU processes. Failure to assess social sustainability at early project stages may lead to development and investment in socially unsustainable technologies. Beyond the UN and GRI approaches Kühnen *et al*. [105] identify:

1. UNEP (United Nations Environment Programme) and SETAC (Society of Environmental Toxicology and Chemistry) S-LCA guidelines
2. SAI (Social Accountability International) SA 8000
3. ISO 26000

The UNEP and SETAC S-LCA guidelines are the most promising stand-alone methodology with respect to the harmonised integration of the three assessment strands. This is largely owing to the influence of ISO 14K on their development, delivering a process modelling approach to data collection and impact identification [106]. The guidelines utilise the same four methodological phases introduced by ISO 14040 (Figure 3-4), supporting harmonisation by providing a common skeleton for assessments. The first iteration of the guidelines was published in 2009 [107], receiving updates through a second version in 2020 to reflect progression within the field. These updates included more detailed methodological guidance, applicability to a wider audience, and attempted resolution of diverging approaches.

Impact indicator application within UNEP and SETAC's methodology follows an analogous approach to most LCA and TEA studies. Potential impacts arising from a project are identified through mid-point indicators. This reduces uncertainty but is necessarily less case specific than the end-point indicators available in LCA (although these are scarcely used) [108]. However, deviating slightly from the methodologies developed for LCA and TEA, indicators are identified through a hierarchical approach. First, stakeholder groups are identified (aligned with the UN SDGs [47]): workers, local community, value chain actors, consumers, children, and society. Notably, practitioners can exclude one or more of these groups if permissible by the assessment's specific goal and scope [106]. Within the stakeholder categories, potential impacts are identified, constituting 'sub-categories'. Each of these can be quantified using several indicators; interestingly, the use of more than one indicator per sub-category is permitted [106]. This approach to indicator selection does ensure that studies utilise a common 'indicator pool', achieving a similar level of standardisation to GCI's TEA guidelines. However, the use of multiple indicators in a single sub-category, or exclusion of others still provides scope for issues, primarily around consistency and comparability between assessments.

Two majorly contrasting schools of thought emerge regarding impact characterisation within social assessments. The reference scale approach, and the impact pathway approach [106]. Reference scale assesses the social performance of a product system through the practices of organisations, examining effects on impact categories. This approach does not typically look at long term effects, a potential limitation in many applications. Conversely, the impact pathway approach uses casual, correlation or regression-based relationships between the product system or organisation and social impact indicators [106]. For methodological harmonisation, the impact pathway approach, involving generation of a process model and data inventories, is the most likely candidate for adoption. This is primarily a result of it being more analogous to the methods seen within LCA. Furthermore, the inventory is assessed with respect to potential social impacts at the mid-point level through characterisation models. The lack of comparable characterisation methods within the competing reference scale approach makes its homologation to LCA and TEA a significant challenge.

3.4.3.2 Current State of SIA in CDU

The progress made towards the standardisation of social impact assessments is visible but still lacking. The EC JRC independently reviewed S-LCA/SIA, determining that it trails LCA significantly in terms of methodological development and standardisation [109]. In addition, Huarachi *et al.* also conclude that SIA cannot be considered a mature field until further development and case study applications are conducted [29]. Furthermore, CDU specific guidelines still prove elusive beyond the integrated framework developed by McCord *et al.* [7] (discussed in Section 3.4.3). Significant progress is required in multiple areas if a standardised approach is to be attained.

Within SIA, qualitative, semi-quantitative, or quantitative data and indicators are present [32] [110], constituting a significant misalignment relative to LCA and TEA approaches. The presence of mixed data types introduces significant complications, primarily around data collection and impact characterisation. These issues are only exacerbated when assessing lower TRL systems, as noted by Rafiaani *et al*. [111]. Quantification of qualitative data should be attempted using expert opinion, focussing on identified areas of importance [111]. Using scoring criteria, this qualitative data can then be applied to a numerical scale, as proposed by McCord *et al*. [7]. However, this naturally incorporates bias and uncertainty, resulting in a secondary issue. While a metric is derived from the application of a scoring scale, a degree of consistency and transparency will be lost, particularly around inter-assessment comparisons. However, this issue may be surmountable if scoring scales can be standardised on a product or sector specific basis.

The consideration and quantification of positive social impacts is another emerging issue within SIA literature [29]. Both LCA and TEA inherently quantify positive impacts (e.g. negative GHG emissions or improved OpEx), requiring resolution for full strand alignment. Importantly, organisations stand to benefit from the inclusion of positive impacts, incentivising further improvements beyond mere legal requirements. Despite this, as of 2020, little progress has been made towards a consensus on the handling of these positive impacts. However, as pointed out by the UNEP and SETAC guidelines, several impact subcategories imply their consideration [106]. One of the major hurdles to overcome is the classification of what constitutes a positive impact. A unified view on this question is a prerequisite to a standardised assessment approach.

To conclude, the evident lack of CDU specific guidance risks leaving complex methodological decisions, such as the specification of assessment boundaries, at the discretion of the practitioner. The GCI's integrated TEA and LCA methodology (discussed in Section 3.4.4.2) should be consulted to attain guidance vicariously when practitioners are confronted with these choices.

3.4.4 Current Integration Efforts

Publications proposing integrated assessments are observed from 2007 onwards; however, they recognise a deep lack of consensus around methodological approach [37] [38]. Tackling these misalignments is a complex proposition, often requiring a trade-off between scientific accuracy and pragmatic decision making support [112]. Such assessments have potential to support a broad range of stakeholders in balancing conflicting goals and positions [74]. Additionally, they deliver a deeper understanding of the economic, environmental, and social trade-offs. In 2017, Zimmermann *et al*. recognised the need for a holistic CDU specific assessment methodology, stating that attainment of such guidelines would allow the systematic evaluation of emerging technologies; ultimately delivering more effective funding allocation and R&D efforts [45]. Specifically, combined assessment could answer broader questions: Is better performance in one dimension worth an offset in the other? And how much better does the performance in one dimension have to be to offset poorer performance in the other?

3.4.4.1 GRI Standards

Aiming to collate the global 'best practices' for public sustainability reporting, the GRI standards [35] can be viewed as a sustainability audit. While considering all three pillars within sustainability, they offer significantly less granular results than many guidelines and standards discussed previously. GRI's standards aim to quantify "the most significant impacts" associated with operation [35], indicating that less coverage will be achieved compared to assessments utilising more tightly controlled and specified cut-off criteria. Furthermore, as identified by Zimmermann *et al*. they target evaluation of deployed activities [45], assessing projects based on real world (deployed) and internal organisation data. This requirement prevents their use in assessments of early-stage projects owing to the inherent inability to evaluate potential impacts.

GRI take a differentiated approach from ISO's standards, contrasting the GCI's homologated LCA and TEA standards. The process model based approach is not present, despite underpinning a majority of methodologies. Instead, identified sources of impacts are grouped under "material topics" (e.g. water and effluents, anti-corruption, etc.); although, no standardised approach is outlined for their selection. These material topics are loosely comparable to the impact categories seen in other assessment strands. Impact indicators, as used by ISO and GCI, are replaced by "reporting metrics". The relevant metrics for assessment are self-determined by the organisation and practitioner, introducing potential for manipulation. Secondly, the number of metrics available for use is vast, significantly hindering comparison between organisations or their technologies. Consequently, resulting assessments may examine the same impacts but employ differing quantification metrics. Some similarities to the ISO and GRI approaches can be observed. For instance, a Shall/Should/May approach is taken to guidance provision, delivering comparable flexibility of application.

Overall, the GRI standards provide a generally robust methodology. However, owing to a variety of reasons, it is not well suited for application to CDU. Assessment of early-stage projects is the largest obstacle. With many CDU projects residing at lower TRLs, a framework that targets deployed technologies or operations is incompatible. Furthermore, CDU requires the assessment of potential impacts, necessitating a degree of uncertainty in the absence of real-world data.

3.4.4.2 GCI Integrated LCA and TEA

Having produced stand-alone CDU based LCA [23] and TEA guidelines [27] (discussed in Sections 3.4.1.2 & 3.4.2.1 respectively), the GCIsubsequently targeted integration. This double stranded thinking delivered the GCIs Integrated TEA and LCA Guidelines, first published in 2018 [39]. These were updated in 2022 along with the stand-alone guidance documents [53]. No other accepted combined LCA and TEA methodologies were found through literature search. Preceding studies instead utilised ad hoc approaches [39].

The GCI approach harmonisation by aligning the goal, scope, boundaries, and assumptions of the individual strands; producing an assessment that is greater than the sum of its constituent parts [7]. While integration is achieved, the GCI ensure that the constituent LCA is still both functional as a standalone assessment and (if desired) ISO compliant. In this approach, the goal and scope phases are unified, with inventory generation and impact analysis conducted in parallel. However, overlapping data inventories permit common data points, reducing the intensity of data gathering while simultaneously improving consistency [53]. This is reinforced by the progress made around CDU specific system boundary specification; targeting pitfalls identified within previous assessments. A key example being the realistic evaluation of CO_2 sources and procurement, a common source of errors leading to overly optimistic assessment outputs.

With the aggregation of the LCA and TEA guidelines, comprehensive integration guidance is now available for practitioners. When compared to ISO 14040 / 14044 or the ILCD Handbook, many methodological decisions have been standardised, unburdening practitioners while improving both reproducibility and validity of results. Despite this, numerous key aspects remain at the practitioner's discretion. A significant example is the selection of impact indicators. It is acknowledged in Section 3.4.1.2 that lacking standardisation here is to ensure broad applicability of the guidelines to CDU projects. However, the challenge remains to define a core set of indicators upon which additions can be made. Integrated assessments add the novel capability of assessing combined indicators, expanding the range of possible insights. Many of these prove to be useful within CDU assessments, with cost of carbon avoided seen regularly within discussion of CDU projects.

The GCI CDU TEA guidelines bring with them the standardisation of many indicator calculation methods, analogous to characterisation models developed for LCA. The harmonisation of these approaches greatly aids their integration. Historically, this has been a stumbling block when comparing TEAs from literature. Attention has also been paid in this area to the broad spectrum of TRL levels observed within CDU. Prescription of alternative calculation methods for technologies at varying degrees of development aids with the difficulties experienced around data availability. The use of contrasting calculations does invalidate comparisons of technologies at different development stages; however, these were already problematic owing to non-uniform development and optimisation efforts.

Offering CDU specific guidance, GCI have advanced best practice within combined LCA and TEA. The result is a highly robust yet broadly applicable methodology, ensuring relevance to all goals and scopes. Where such double stranded assessments are necessitated (e.g. applications for financial capital), it should be considered the benchmark. Furthermore, the case studies provided, along with the Shall/Should/May guidance provision, facilitate use by relatively inexperienced practitioners.

3.4.4.3 The Triple Helix Framework

Published in 2021, the Triple Helix Approach developed by McCord *et al.* [7] is the first CDU guidance to consider all three strands of sustainability in parallel. This is realised through the development of an SIA strand that is compatible with the existing ISO homologated TEA and LCA guidelines; delivering a well-integrated assessment when performed together. Given their already advanced state and CDU focus, the GCI's Integrated TEA and LCA guidelines are an ideal foundation for the addition of the third SIA strand.

In contrast to most social assessment methodologies, the framework aligns the SIA's focus around the process and its deployment rather than the organisation itself. The proposed methodology is recognisably based on the UNEP/SETAC guidelines, inherently providing a degree of alignment with ISO's LCA standards [55]. Consequently, the four phases seen in LCA and TEA (Figure 3-4) are once again employed.

Data collection is recognised as a major hurdle for social assessment. McCord *et al.* structure the methodology around the use of open-source data, facilitating use by a wider practitioner base; recognising that utilisation of organisational data makes assessment impossible for outside third parties. Due to the low TRL of many CDU projects, data is often unrepresentative of the deployed iteration of the process. Despite supporting supply chains often being fully developed or deployed [7], they are regularly opaque, making the tracing of materials to extraction a challenge. Consequently, SIA indicator calculations usually yield 'fuzzy' results with significant degrees of uncertainty. However, insights into the surrounding potential social impacts remain attainable. Much of the required data is shared with the parallel LCA and TEA (mass and energy balances, workforce requirements, etc.), reducing practitioner workloads. Additional data is required in the form of geographically specific data evaluating indicators such as child labour and forced migration.

Developing a novel approach, McCord *et al.* determines key indicators for CDU social assessments; and approaches to their calculation. The framework adopts the UNEP/SETAC selection process, although removes several stakeholder categories due to reduced relevance within CDU. The presence of qualitative data often hinders the application of characterisation models to generate quantitative indicator results. Consequently, an approach is developed for the conversion of this qualitative data to quantitative. In the triple helix framework, practitioners derive a reference scale for each indicator, requiring experience and knowledge when assessing the system. A five- or nine-point scoring scale is recommended to ensure the correct level of granularity and differentiation [7]. While practical, this approach carries some risk of inconsistent scoring, resulting from the degree of practitioner involvement. Furthermore, there must be consensus around whether a high or low score is favourable; this must be uniform across a given assessment. Despite employing these practices, many indicators evade expression in terms of a functional unit, presenting a persistent issue around the integration of assessment strands.

The indicators present within integrated assessments generate potential conflicts. For example, high wages would be positive from a SIA stance, yet detrimental from a TEA perspective [109]. Opposing views are present on whether this constitutes a methodological issue. While making optimisation difficult, particularly with respect to deployment scenarios, it facilitates greater understanding of inter-strand performance trade-offs; one of the primary motivations for the development of integrated assessments. [7] This characteristic of combined assessments is flagged within the triple helix but the addition of conflicting indicators is not discouraged, helping to reflect complex real-life impact interactions.

In summary, while offering a significant advancement for CDU SIA, several methodological issues persist; primarily concerning standardisation. The most notable example is calculation of impact indicator results. Despite offering a method of pseudo-quantification, the scoring scale approach prevents comparisons between assessments in literature. The issue is complex to resolve due to the breadth of assessment goals and scopes. However, if the scales for commonly employed indicators can be standardised, potentially using world ranking data, the comparability difficulties may be alleviated. Given the timeframes required to reach and adopt accepted characterisation models in both LCA and TEA, it should be expected that such approaches are multiple years away for SIA.

Guidance is also lacking around the specification of system boundaries. Developed to be compatible with the GCI combined TEA and LCA guidelines, the SIA boundaries should be defined accordingly. However, social impacts are, in many ways, more complex than their environmental or economic counterparts. The introduction of a new process plant or supply chain to a region may affect a plethora of peripheral stakeholders, acting through mechanisms such as access to energy or material goods. Further guidance around boundary rules or cut-off criteria would aid resolution.

The infancy of CDU SIA and the associated methodological shortcomings are recognised as a significant hurdle by the triple helix framework [7]. It is proposed that the framework receive further development through repeated application and refinement. This first iteration is deliberately broad, allowing for further adaptation around specific CDU needs. Given that development targeted a 'framework', it could be argued that the provision of further practitioner support would result in a transition towards guidelines. Despite the advantages of this wide applicability, it does result in the need for significant practitioner experience and expertise, particularly around impact analysis. Substantial further development is need in the CDU space to remove this barrier and encourage widespread use.

Despite unavoidable limitations within the first iteration of an assessment framework, multiple insights were revealed. The most significant being the identification of raw material sourcing as a key hotspot for social impacts around CDU projects [7]. Secondly, cascading impacts associated with the use of large quantities of renewable energy; for instance, green H_2 production often significantly impacts the surrounding community and society. Recognition of these broader impacts will be critical in the examination of Power-to-X processes within CDU, ensuring a "just transition" towards sustainability.

3.5 Discussion

Critical review of the current literature around CDU assessment reveals that the Triple Helix framework, in conjunction with the GCI guidelines, delivers the greatest degree of both holism and harmonisation. Released in 2021, a 14-year gap can be observed between the first calls for a harmonised methodology and its realisation. The partial alignment of the social strand with GCI's ISO compliant combined LCA and TEA delivers a first of a kind sector specific triple stranded approach.

Progress towards a harmonised and holistic approach to CDU specific sustainability assessment can be charted through examination of the guidelines identified. When viewed chronologically, this generates a 'taxonomy' (Figure 3-9), detailing the lineage from which the triple helix approach hails. Of clear significance is the dependence of all strands on the ISO 14040 / 14044 standards. These documents have come to form the backbone of most subsequent approaches, primarily in the form of assessment structure.

While the taxonomy omits standards, guidelines and frameworks that do not directly contribute to the triple helix framework, the bias of methodological development towards LCA is clear. This is an unsurprising discovery given its status as the oldest assessment strand, hailing to the 1960s [18], and the only strand with an ISO standard (at the time of writing). The first attempt at TEA standardisation is both CDU sector specific and surprisingly recent, published in 2018 [22]. While TEAs have been conducted on scale (as shown by Figure 3-7), lack of standardisation is surprising given their ability to identify economic efficiency gains. It can be seen from TEA's representation in Figure 3-9 that the absence of standards is not necessarily indicative of a low count of assessment applications. SIA is found to be the least developed strand, as other non-CDU specific reviews have concluded

[45] [30] [31] [32] [29]; implying that the observed phenomenon is inter-disciplinary in nature. A first attempt at CDU specific SIA guidance was absent until 2021, with standardisation of application still lacking.

The triple helix approach provides practitioners with guidance on the application of SIA within combined assessments. For this reason, it will subsequently be considered the best practice in SIA, particularly for full studies concerning final selection of CDU projects. The TEA strand is best represented in the field by GCI's guidelines [27], owing to its sector specificity, ISO compliance and structural harmonisation.

The degree of overall harmonisation achieved around holistic sustainability assessments is therefore assessed based on the GCI's LCA and TEA guidelines [23] [27], and UNEP / SETAC's SIA guidelines [106]. Given their homologation to the same four phase assessment format, the constituent components within their goal and scope requirements can be compared. The findings are shown by Table 3-3 and Table 3-4.

Table 3-3 - Goal requirements for independent strand assessment methodologies [23] [27] [106]

		Assessment Strand		
		LCA (GCI)	TEA (GCI)	SIA (UNEP/SETAC)
Goal Component	Context	✓	✓	✓
	Intended Application of Findings	✓	✓	✓
	Intended Audience	✓	✓	✓
	Commissioners and Practitioners	✓	✓	
	Motivation for Assessment	✓	✓	✓
	Use for Comparative Assertions	✓		✓
	Limitations of Assessment	✓	✓	
	Stakeholders Affected			✓

As shown by Table 3-3, GCI's guidelines for CDU based LCA and TEA assessments are almost fully aligned. The only exception to this is the requirement to state whether the study will be used for comparative assertions. Clearly, this will not be problematic if incorporated within a TEA assessment, thus facilitating total alignment of study goals. Comparative assertions are less common within TEA studies as their application is usually for internal commercial use, incorporating sensitive data that prevents external communication. However, the context of the TEA must still be covered, giving insight as to whether the study is comparable to others, this details the assessed location, time horizon, scale, and commercial partners [27].

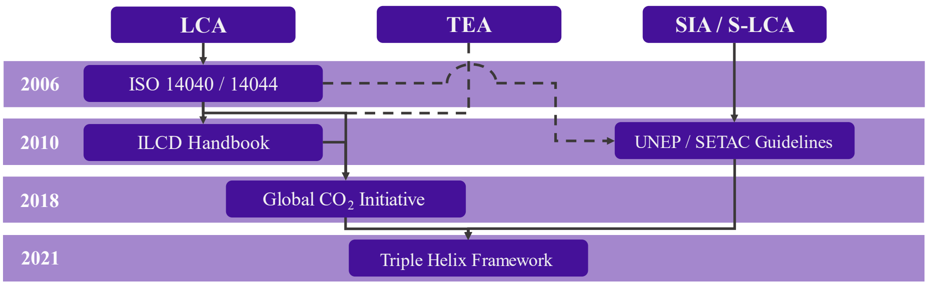

Figure 3-9 - Taxonomy of standards, guidelines, and frameworks leading to a holistic environmental assessment framework for CDU applications. This figure excludes contempory methodological developments that were not directly utilised.

Once again using GCI's LCA guidelines as the benchmark, the SIA strand can be seen to exhibit a moderate degree of alignment. The requirement to state the stakeholders affected reflects the strands interest in human societal impacts. In contrast to LCA and TEA, the stakeholders affected are not limited to the commissioner and intended audience. Furthermore, the limitations of a given study are not defined within the goal. Instead, details of these reside within the assessment's scope. Due to their inclusion, albeit elsewhere, the SIA strand is only deemed to be partially misaligned in this respect.

Unanimously, the assessment scopes contain more information than the goals; a legacy of ISO 14044. As a partial consequence, a lesser degree of alignment is observed. As the most established and employed assessment type, LCA will once again be used as the benchmark for comparison.

Table 3-4 - Scope requirements for independent strand assessment methodologies [23] [27] [106]

		Assessment Strand		
		LCA (GCI)	TEA (GCI)	SIA (UNEP/ SETAC)
Scope Component	Study Context		✓	
	Functional Unit	✓	✓	✓
	Reference Flow	✓	✓	✓
	System Boundary Definition	✓	✓	✓
	System Boundary Flow Diagram	✓	✓	
	Completeness Requirements	✓	✓	✓
	Cut-off Criteria Applied	✓	✓	✓
	Inventory Structure	✓		✓
	Allocation Procedure	✓		✓
	Data Quality Requirements	✓	✓	✓
	Defined Product Function		✓	
	Selection of Benchmark System		✓	
	Assessment Limitations			✓
	Approach to Impact Assessment			✓

LCA and TEA are largely aligned, sharing ~78% of the components present in LCA's scope, with TEA exhibiting two additional requirements. Of these, the most pertinent is the definition of a benchmark system, arising from the typical application of TEA to assess the benefits of a process or system against an existing or deployed one. LCA studies are occasionally conducted without a benchmark system, aiming to quantity potential impacts of a technology in isolation. For combined assessments a benchmark should be encouraged to maintain the level of insight generated by standalone TEAs. Other discrepancies are present, including specification of allocation procedures, definition of product function and inventory structure. For combined LCA and TEA, these are relatively easily aligned, often with no alteration to methods. However, the selection of allocation procedure may be impacted by integration, requiring a harmonised approach. This may result in a compromised strand, caused by selection of a locally non-ideal allocation approach. For example, inclusion of TEA is likely to favour economic allocation, a less desirable option within LCA (as confirmed by ISO 14044's hierarchy) [56].

SIA shares ~89% of the scope requirements present for LCA, a surprising amount given the strands lagging maturity. The only component not mirrored from LCA's scope is the definition of a system boundary flow diagram, required by LCA and TEA. This is a result of the inherently qualitative nature of social assessment and uncertainties within the impact chain. Despite this, the parallel presentation of a system flow diagram is not a source of incompatibility, potentially enhancing the identification of social impacts. The additional aspects required are assessment limitations and the approach to impact assessment. Limitations are covered within the goal for both LCA and TEA. For a combined assessment this is easily resolved through aligning the positioning of limitation evaluation. The second and more complex addition is the specification of an approach to impact assessment. As discussed in previous sections, the characterisation models seen within other assessments, particularly LCA, are absent from SIA. This leaves much broader methodological scope for the quantification of impacts. The triple helix approach [7] offers perhaps the most robust approach to the handling of qualitative data. However, still elevates uncertainty relative to the two other strands.

Moving away from the requirements of goal and scope setting, the more general state of alignment can be considered. The three emerging assessment methodologies, examined for Table 3-3 and Table 3-4, utilise fully harmonised assessment structures; based on ISO. Critically, this enables the further alignment of constituent aspects for each phase. TEA and LCA are easier to homologate, owing to their sole reliance on quantitative data, generating the already noted challenge for SIA alignment. While constituent assessment phases are now common across all three strands, the methods employed within them vary, sometimes significantly.

Indicator characterisation is the largest source of divergence within integrated assessments. The level of standardisation achieved follows the trend of general strand maturity. LCA provides well defined indicators and standardised characterisation models [113] [70] [114], delivering comparable methodologies even in the absence of aligned boundaries or assumptions. TEA is less refined; however, GCI deliver CDU specific guidance on the characterisation of commonly used indicators [53]. The recommended methods are stratified in accordance with TRL levels, preventing comparison between TRLs but augmenting accuracy as technology maturity increases and data quality improves. This is, in most cases, a favourable approach due to the complexity of comparing differing TRL technologies; usually requiring the application of learning curves and highly uncertain scale-up considerations.

Overall GCI deliver a largely analogous approach to LCA, incorporating current best practices throughout the TRL range. In contrast to this, UNEP/SETAC provide a significantly less developed approach. While outlining suggested indicators, there are many more than are observed in other strands, spanning a total of 30 categories [106]. Furthermore, their characterisation evades standardisation, hindering sector wide and comparable methodologies. This is largely caused by the presence of mixed data types; a problem that is partially resolved by the triple helix framework [7]. However, despite its application of scoring scales for indicator quantification, they must be standardised for satisfactory resolution of the problem.

Precursing this, the selection of impact indicators for evaluation is another common source of divergence between otherwise comparable assessments (both independent and integrated). A ‘standard’ selection of indicators to assess within each strand would, on the surface, greatly benefit integrated assessments. However, this is a similar approach to that taken by the PEF Category Rules [57]. As PEF demonstrated (discussed in Section 3.4.1.2), rigid prescription of indicators hampers the application of assessment guidelines to sufficiently broad ranges of goals and scopes. For LCA and SIA, standardisation within sector level guidelines, such as CDU, is impossible. Different CDU processes and products will involve different environmental and social impact pathways and effects, requiring a tailored selection of assessment indicators. TEA is the most promising opportunity for standardised indicator selection. Economic sustainability primarily rests upon OpEx, CapEx and product market prices, as supported by GCI's analysis [22]; assessment of just these factors would likely provide serviceable insights.

Resolution within assessment results has been safeguarded throughout strand integration by the consistent adoption of ISO's process flow diagram approach to system modelling. This encourages the generation of data inventories around individual process aspects. For 'technical-level' assessments of processes this is the constituent unit operations; whereas for supply chain focussed, or 'corporate-level' assessments, whole processes may be considered. Consequently, the granularity of detail obtained from assessments is primarily determined by the assessment scope and practitioner's workload restrictions. In this area GCI make significant contributions. Utilisation of a shared inventory between strands reduces the complexity of the LCI phase, allowing for increased focus on areas such as cut-off criteria or enhanced impact characterisation. This approach is supported throughout the triple helix approach, suggesting that shared mass and energy balances from the LCA and TEA form the backbone of the SIA inventory.

Across all guidance documents, allocation remains unstandardised representing one of the largest remaining sources of practitioner influence. While a methodological hierarchy is presented by ISO, and retained by most subsequent frameworks, the selection of approach must ultimately reflect and service the proposed goal and scope. Consequently, it is unlikely that a resolution will be reached in this area, necessitating transparency around the method employed. Alternatively, the standardised reporting of the mass and energy balance alongside the allocated indicator results will allow practitioners to latterly distribute impacts via an alternate approach. While this would greatly enhance the data availability in literature, many organisations would likely oppose the public disclosure of their process operations on the basis of commercial sensitivity.

Comparability between assessments, characterised by the 'apples vs oranges' problem identified by Zimmermann *et al*., has improved incrementally but consistently. Each guidance document on the path to a harmonised CDU assessments (shown by Figure 3-9) delivers more specific practitioner guidance, resulting in fewer methodological decision and therefore divergence. The PEF Category Rules provide the most comparable studies, rigorously specifying almost all decisions on behalf of practitioners. However, as discussed, this hinders harmonisation with other stands. GCI deliver, for CDU projects, an exemplary level of guidance, limiting divergence while remaining relevant to broad varieties of goals and scopes. This partial constriction of methodological choices has the added benefit of enhancing study robustness through the reduction of erroneous methodological choices. Unsurprisingly, SIA exhibits a less constrained methodology compared to the other strands or methodologies. This is likely an inevitability within social assessments, precipitating from difficulties around boundary setting and the accurate tracing of impact pathways; both preventing intricate and standardised assessment procedures.

Significant gains could be made around combined assessments if more comprehensive databases were generated for the TEA and SIA strands. Currently LCA monopolises on practitioner databases, with Ecoinvent being the most commonly employed. The technical data within TEA makes such collation difficult, with many studies focussing on novel processes for which data is not publicly available. However, aspects of the assessment, for example commodity and feedstock market prices, could be collected. If such data was organised by date, region and material specification, large comparability and quality improvements would be seen. SIA, however, is much more complicated. While broad data, likely country specific, could be collected; including slave labour, gender equality, safety standards, etc, it is unclear how this would be directly integrated to either the UNEP/SETAC or triple helix framework.

3.6 Conclusion

In conclusion, the three strands of assessment have achieved remarkable levels of harmonisation since 2007 when integrated methodologies were initially conceived. ISO's 2006 publication of LCA standards form the basis of development. GCI's subsequent generation of the first CDU specific guidelines successfully aligned both LCA and TEA, receiving broad acceptance. However, the final stage in harmonising CDU specific assessments continues to represent significant challenges; the alignment of SIA. Successful first steps have been made in the form of the triple helix framework; however, the strand lags behind its environmental and economic counterparts. Consequently, SIA cannot yet be deemed to have achieved a satisfactory degree of harmonisation.

As a result of its failure to reach maturity, CDU SIA is currently relegated to primarily 'red flag' applications. In this capacity it can successfully identify potential sources of unsustainable social practices; however, remains vague and unprecise. Until the tracing of impacts and characterisation methods can be improved, full harmonisation is unlikely to be realised. Given the time periods required to generate this knowledge for LCA, attainment of such models is likely some years away. This presents practitioners with a dilemma within the CDU space; should SIA be implemented as a complimentary strand on a 'red flag' basis, or discarded from assessments?

Differing schools of thought percolate within the community; however, a majority identify SIA as a critical component of holistic assessment. Practitioners are subsequently faced with selecting a mode of assessment application. From the literature reviewed, SIA appears suitable as an assessment 'screen'. Application in this capacity, as indeed proposed by McCord *et al.*, plays to the strength of lacking data availability; providing a go-no-go verdict on the value of further work and time intensive assessment. If successful, a system can then be evaluated on the basis of GCI's integrated TEA and LCA guidelines. If possible, at this stage, a more detailed iteration of the SIA should also be completed; again, using the triple helix framework's approach. Following this assessment pattern, a holistic overview of the systems sustainability profile is attained, with a respectable degree of methodological harmonisation between strands.

If a 'just transition' towards sustainable society is to be achieved, SIA cannot reasonably be relegated into a second strata of assessment. At the very least, application in its current form will prevent R&D efforts and economic investment into fundamentally unsustainable processes, systems, or supply chains. In many senses, this alone should be seen by industry, policy makers, and the public, as invaluable. Future work in the field should focus on the iterative improvement of SIA within integrated CDU sustainability assessments, using the triple helix framework as a competent first step. As discussed, many methodological aspects would benefit from greater degrees of standardisation, most notably impact quantification methods, or agreed upon scoring scales.

3.7 Additional Evaluation of FMCG Value Chain Relevant Guidance

To supplement the literature review of CDU oriented assessment guidelines presented in this chapter, a brief review of FMCG relevant counterparts was deemed necessary. Consequently, literature searches were conducted on Web of Science, in line with the approach used previously in this chapter, to identify relevant practitioner guidance documents. Search terms of 'LCA', 'Lifecycle Assessment', 'TEA', 'Technoeconomic Assessment', 'SIA', and 'Social Impact Assessment' were used, with the additional requirement that the term 'FMCG' or 'Fast Moving Consumer Goods' was present in the title, author keywords, or abstract. This was enforced to ensure that returns were based on methodological development or guidance, as opposed to individual publications taking ad hoc approaches to specific product or value chain oriented assessments. Methods for assessing competing pre-deployment FMCG value chains were of particular interest, reflecting the needs of Unilever's Clean Future initiative in which novel value chains must be selected or recommended from a large number of alternatives. The nature of this assessment goal requires detailed consideration of globalised value chain structures, feedstock procurement route variety, high throughput rates, consumer behaviour variability, and in the case of cradle-to-grave assessments, packaging waste implications.

Despite ensuring no additional constraints were in place, the previously listed search terms returned no FMCG specific guidance documents for the LCA, TEA or SIA assessment strands; a direct contrast to the previous search for CDU based literature. Despite this, two publications were returned focussing on the potential value addition of LCA or TEA application within the FMCG value chain context. No publications were returned for FMCG oriented SIAs.

3.7.1 FMCG Oriented LCA

A detailed earlier in this chapter, ISO 14040 and ISO 14044 provide practitioners with the fundamental methodological principles and requirements for the conduction of LCAs. These are broadly applicable and have been extensively deployed across all major industrial sectors [21]. In the context of FMCGs, LCA offers the opportunity to identify environmental hotspots within upstream and downstream supply chain components, or processes under the direct control of the FMCG company. However, this hinges, particularly for upstream aspects of the supply chain, on the transparency of suppliers and the availability of process data (be that primary or secondary in nature); both of which are common stumbling blocks within the LCI phase is assessments involving corporate entities [115].

Currently, standards and guidelines do not provide any FMCG specific support for practitioners. While this can be circumnavigated in assessments of existing deployed value chains by modelling the value chain as a classical system, such a solution is not as straightforward for the comparative assessment of pre-deployment scenarios. As discussed above this necessitates additional context specific considerations. The lack of practitioner guidance for future looking FMCG value chain development risks exposing the field to assessments with incongruent system boundaries, inappropriate impact allocation procedures, or improper functional unit selection. Consequently, a FMCG equivalent of the GCI's CDU LCA guidance [39] would both improve the comparability of assessments and ensure that study results are representative of potential real world deployments.

Identified briefly within the review of CDU LCA guidance, the PEF category rules partially resolve the guidance issue in limited specific scenarios. While not broadly tackling assessments of FMCG value chains, several key products from Unilever's product portfolio are covered, for example: liquid laundry detergents, pet food, and packaged water. While potentially useful for development of these product's future value chains, they are highly specific and cannot be easily translated to different product types. Furthermore, the PEF category rules are highly constrained methodologically in terms of indicator selection and reporting format; while useful in many applications it severely restricts the range of questions that can be answered through their use [19].

One returned paper examined the application of LCA to characterise the impacts of transport steps within FMCG value chains [116]. While of value during the optimisation of FMCG value chains, the paper offers no guidance beyond transport steps, severely limiting its utility to practitioners looking to assess full systems. The second of the papers returned by the literature search, written by van Elzakker, *et al*., considered the role of LCA and TEA in the optimisation of existing FMCG value chains [117]. The work highlights a previous focus on TEA assessments for the optimisation of FMCG value chains, neglecting the value addition of a parallel LCA. However, it is also noted that pressure from regulators and NGOs have resulted in the incorporation of some environmental objectives within the FMCG value chain optimisation process, resulting in a discipline referred to as Green Supply Chain Management (GrSCM). This assessment approach was subsequently examined by Srivastava [118], Grossmann and Guillén-Gosálbez [119], and Hassini *et al.* [120], all identifying issues regarding the definition of independent environmental indicators that do not incorporate economic aspects, and around the systematic balancing of trade-offs between assessment strands. If meaningful comparative assessments of pre-deployment FMCG value chains are to be realised, issues such as these must be resolved through application specific methodological guidance.

3.7.2 FMCG Oriented TEA

As discussed in detail within evaluation of CDU guidance, TEA is generally less methodologically standardised than LCA. However, several TEA guidelines exist that are of partial relevance to the assessment of FMCG value chains, particularly in the context of purple carbon and Unilever's clean future initiative; primarily the CDU oriented guidance from the GCI [39].

The FMCG sector, being inherently reliant on dynamic, cost-sensitive, and high throughput operations, necessitates a tailored approach to TEA. This is likely to require a modular approach that incorporates supply chain structures and logistics, regulatory compliance, and cost trade-offs between competing feedstocks; all of which are required if the sector is to make meaningful and efficacious progress towards the attainment of sustainable industrial ecosystems. While the GCI's CDU-oriented TEA methodology offers a foundation for this type of economic assessment, they require significant further refinement in terms of inventory structure to address the large number of competing feedstock types and sourcing routes demanding parallel assessment.

3.7.3 FMCG Oriented SIA

The UNEP and SETAC guidelines currently provide the most structured methodology for evaluating social impacts as fully outlined within the previous review of CDU guidance. Since the release of these guidelines, no additional sector specific granularity has been achieved. The closest observed approach to FMCG specific SIAs is found in the Handbook for Product Social Impact Assessment [121], published contemporaneously to the UNEP and SETAC guidelines. However, this assesses only select parts of non-FMCG specific product lifecycles with a constrained list of indicators, ultimately delivering results in the form of a reference scale, as seen in the Triple Helix Framework of McCord, *et al.* [7]. Consequently, the methodology is not truly FMCG specific, or capable of fully and comparatively assessing value chains on a cradle-to-gate or cradle-to-grave basis. Furthermore, the utilisation of reference scales results in reporting against a discrete values that are incongruent with the typically continuous nature of LCA and TEA reporting methods, requiring the development of impact pathway based social impact characterisation models.

Given the global reach and large workforce requirements of typical FMCG value chains [122], SIA has the potential to offer valuable insights around impact hotspots, pathways, and severity. However, this is currently prevented by the aforementioned methodological shortcomings; a potential consequence of the strands relative youth compared to LCA and TEA. To realise valorisation of the assessment strand, existing SIA guidelines must be augmented to better address the unique requirements and challenges faced by FMCG companies during their transition towards sustainable operations.

3.7.4 Overview of Sustainability Assessment in the FMCG Context

The absence of comprehensive FMCG sustainability assessment guidelines across all three strands results in methodological gaps and challenges, significantly constraining and hindering the conduction of large scale comparative or prospective assessments within the sector. One of the most pressing challenges is the absence of tailored LCA guidelines for FMCG value chains, with the environmental strand typically being the first mover towards new sector specific guidance. Despite the broad applicability of ISO 14040 and ISO 14044 standards, these frameworks fail to accommodate the unique complexities of FMCG operations, particularly for pre-deployment value chain development. The partial applicability of the GCI’s CDU guidelines and the Product Environmental Footprint (PEF) category rules provides limited assistance, but remains highly constrained in scope, failing to offer methodologies applicable for use across FMCG product portfolios. Development of a robust FMCG LCA framework would significantly aid in the subsequent development of TEA and SIA counterparts.

A similar set of challenges observed within LCA extend to FMCG specific TEA guidance, with the sector requiring a modular and context-specific approach to pre-deployment assessments. While existing TEA methodologies provide a strong and robust foundation, they lack the granularity required to repeatably navigate the FMCG-specific supply chain structures, logistics, and regulatory constraints that commonly result in divergent practitioner decisions [53]. The absence of structured and modular inventory frameworks, capable of accommodating a diverse range of feedstocks and sourcing routes, currently represents the most significant barrier to impactful TEAs of pre-deployment FMCG value chains.

SIA presents the greatest challenge of the three assessment strands. Existing methodologies, such as the UNEP and SETAC guidelines and the Handbook for Product Social Impact Assessment, while methodologically robust, fail to fully capture the nuances of FMCG value chains. Reliance on reference scale impact characterisation and reporting methods render previous frameworks incongruent with the needs of FMCG companies and existing LCA and TEA approaches.

In conclusion, while LCA, TEA, and SIA offer fundamental and important insights into the sustainability of FMCG value chains, their current and historical methodological limitations prevent their effective use. To advance sustainability assessment in the FMCG context, a comprehensive and tailored methodology must be developed to address inventory structure. Furthermore, to realise holistic assessments capable of evaluating burden shifting, the methodologies for the environmental, economic, and social strands must be harmonised in terms of reporting.

4 Assessment Architecture Development

The work within Section 4.5.2 of this chapter has been published within Frontiers in Energy Research:

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Contribution Statement (pertaining only to the included section):

Alex Newman - Conceptualization, methodology, formal analysis, investigation, literature and data curation, writing, review and editing.

Peter Styring - Supervision and review.

4.1 Introduction

Sustainability assessment is, and will continue to be, a highly coveted tool within industrial development. Many complex and interconnected question can be answered through its proper application and conduction. For instance, should investment be made in process plants to produce bulk chemical domestically in the country of use? Or, might it be more sustainable to manufacture elsewhere where renewable energy is more readily available and transport the finished product to the use market? Such examinations of complex value chains necessitate a holistic approach to impact evaluation, and more broadly, assessment structure. It is therefore clear that, in the setting of sustainable industrial development, the persisting dogma of isolated environmental, economic, and social impact assessments fails to capture important nuances and is no longer fit for purpose.

Within this section a novel and holistic sustainability assessment framework is developed, laying the groundwork for subsequent application and testing. An overarching schematic is presented along with the specification of pertinent methodological choices. In a fashion comparable to the ISO 14040 standard's key principles, a guiding philosophy is laid out, based on which methodological techniques are selected, and guidance is prescribed [55]. Some constituent aspects draw heavily from previous attempts at integrated assessments, while simultaneously augmenting their capabilities and buttressing weaker aspects. A focus is also placed upon the direct re-use of assessment LCIs in subsequent studies, in theory, delivering workload reductions with repeated framework application.

The work has been carried out in the context of sustainable value chain development within a FMCG company, aiming to offer resolutions to many of the persisting gaps in capability previously identified in Chapter 3. To this end, an initial analysis of a typical FMCG company's sustainability assessment based requirements is undertaken, facilitating the development of appropriate methodological techniques and delivery of a more utilitarian and application specific assessment structure. This generated knowledge forms the foundation around which the overall framework is subsequently constructed, providing industrial decision makers with a bespoke and approachable tool.

As part of this tailoring to FMCG use cases, MCDM is incorporated to allow for the consideration of value choices to quantify the relative importance of the included impact indicators; ultimately, this should allow for progress towards sustainable industrial ecosystems in alignment with broader corporate strategies or values. While this adds a subjective element to the assessment's results, a fact recognised in previous work [7], this is counterbalanced by the requirement to present traditional objective results in parallel. This requirement safeguards against 'greenwashing' and enforces accountability for any decisions precipitated from the assessment results.

Due to the targeted application within industrial and corporate settings, the assessment is sub-divided into two sections. On the more technical level, practitioners are required to 'feed' the framework with robust LCI data, ensuring that aspects such as the system boundary, impact characterisation, and data quality requirements are handled correctly and consistently. The second, more general level, caters to decision makers and non-practitioners. It includes the systematic input of impact indicator-based value choices, generating a pared back and actionable summary of the value chain's impact and enhancing interpretability.

4.2 Aims and Objectives

It should be recognised that the aims and objectives for this section of work are qualitative in nature, a consequence of the focus on methodology and theory. However, these theoretical benefits are tested in practice within the proof-of-concept chapter presented later (Chapter 6). In essence, the aim of this work is to develop and present a holistic value chain oriented sustainability assessment framework that meaningfully incorporates decision maker value choices while safeguarding the provision of robust objective impact indicator results.

Table 4-1 Objectives of Chapter 4.

Objective	Specification
2.1	Specification of a guiding philosophy for framework development that is aligned with the values of the ISO 14040 standard.
2.2	Identification of attributes required for the meaningful application of holistic sustainability assessment within the context of a fast-moving consumer goods company.
2.3	Selection and integration of an appropriate and robust multi criteria decision making technique to facilitate the ranking of available value-chains.
2.4	Development of a standardised data input format, allowing for re-use of lifecycle inventory and analysis data.
2.5	Development of a FMCG value chain oriented assessment architecture capable of holistically and objectively assessing a broad range of systems while simultaneously ranking the available alternatives against decision maker value choices.

4.3 Guiding Philosophy

As discussed, the assessment strands have historically been evaluated in isolation. However, more recently value has been recognised in the development of integrated methodologies, allowing for the parallel evaluation of the strands under a single assessment format [46] [39] [123]. Meaningful and seamless integration relies heavily upon the success of underpinning methodological harmonisation efforts around the four-phase assessment format developed within the ISO 14040 standards. If the methodological phases and approaches exhibit large variation, such as the use of qualitative as opposed to qualitative data, cross-linkages are difficult to establish. Common or modular data inventories should be targeted within integrated frameworks, improving both reproducibility and required workload.

Where feasible, methodological decisions should also be harmonised across the assessment's strands, examples being the setting of combined goal and scope statements, functional unit selection, etc.; however, this is not always the case. For instance, within the triple helix framework, McCord, *et al*. examine the use of 'eco-enviro' indicators [7]. In contrast, this work proposes that the use of independent indicator sets for each of the three assessment strands is more efficacious, allowing for a more nuanced understanding and quantification of burden shifting. As an example, OpEx and GWP are often assumed to be strongly and negatively correlated [124]. When evaluated over a range of alternative systems, using stand-alone indicators, this can be accurately confirmed or nullified. This operationalises a primary strength of holistic approaches; the ability to identify three-dimensional burden shifts. When used to inform investment in R&D efforts, it is important that negative impacts are not just optimised within a single area; often sustainability requires complex trade-offs and compromise that cannot be fully summarised qualitatively.

While the triple helix largely harmonises SIA to the GCI LCA-TEA guidelines, data remains problematic with the juxtaposition of qualitative and quantitative impact characterisation. In this research, the common LCA and TEA data inventories, already realised by the GCI [39], are augmented to include the quantitative data and impact characterisation procedures required for complete harmonisation of the societal strand. Previous to this, the deployment of practitioner-led reference scale approaches delivered pseudo-quantitative social impact indicator results relying on practitioner judgement. Therefore, leading to less robust and reproducible results. Development and incorporation of SIA characterisation models analogous to those observed in LCA facilitates repeatable comparison of systems across all three strands.

LCA, and sustainability assessment more broadly, is a notoriously complex and data intensive field to study [125]. This fact typically makes the results of assessments less approachable to corporate decision makers who are often non-practitioners. A challenge is therefore revealed; how can the results of a holistic assessment be communicated most effectively? An obvious solution is the incorporation of a decision-making tool that can condense the assessment's results into a single overall score that simultaneously considers the organisations strategy and values. However, this approach unavoidably adds subjectivity, a historical adversary of LCA practitioners. To combat this, any adoption of decision-making support of this type must occur in parallel to the traditional assessment structure, safeguarding the objective results.

Despite the foundations for complete integration being present, several details continue to divide opinion. For example, the assessment and balancing of conflicting indicators adds subjectivity to the results [7]. The question must be posed: at what point are improved environmental impacts negated by increased OpEx or CapEx? Or balancing high working wages with OpEx? Assessment strand integration generates multivariate problem spaces that are complex to optimise. While again unavoidably adding subjectivity to the decision-making process, it is reflective of the reality of the transition to a sustainable society and industrial ecosystems, necessitating and justifying evaluation.

Philosophically, the process of developing an assessment framework should focus on delivering maximum utility and efficacy to both users and stakeholders. Consequently, key methodological aspects, such as the network's topological structure, and MCDM technique, are initially selected based on their fitness for purpose in the context of FMCG value-chains. Only once these framework 'modules' have been identified is their assembly into a functional architecture considered. This ensures that the most appropriate approaches are included at each step of the assessment, avoiding decisions based purely on convenience. Such developmental shortcuts can be seen through the lack of repeatable impact characterisation methods within counterfactual approaches observed in literature [126].

These key differentiators from existing methodologies contribute to safeguarding the idea of a 'just transition', ensuring progression around sustainability is available to all. The inclusion of a quantified social strand is key in preventing the often-unseen negative side-effects of progress towards environmental sustainability.

4.4 Achieving Utility Within the Setting of a Fast-Moving Consumer Goods Company

FMCGs represent a very specific application case for sustainability assessment. Typically, the FMCG is a large player within its associated value chains, requiring vast amounts of internal re-working and manual handling of complex data sets [127] in order to realise benefits in any of the three strands of sustainability. A 2022 report, compiled by the Consumer Goods Forum (CGF) and Ernst & Young (EY), determines five factors pertinent to FMCG companies achieving the 2030 United Nations Sustainable Development Goal targets [128]:

1. Partner for success - Profitability and revenue competition are part of a healthy economy but solving sustainability's systemic challenges requires collaboration.
2. Measure progress and impact - Businesses can't manage what they don't measure – and there is a clear need to integrate the SDGs with internal frameworks.
3. Embed sustainability into the corporation's DNA - Companies that embed the sustainable into their culture are far more likely to achieve them.
4. Bring the consumer on the journey - Consumers are rewarding those businesses who do the right things to improve the health of communities. If businesses fail to act on urgent environmental and social issues, they will get left behind.
5. All SDGs should be supported but prioritize the areas where you have the power to make the biggest difference - certain companies can make a greater contribution to some SDGs than others, depending on their experience and sphere of influence.

These factors were identified through consultation and interviews with the CEOs of thirteen of the largest FMCG companies, including; Unilever, Ahold Delhaize, Alibaba Group, Ajinomoto Group, A.S. Watson Group, The Coca-Cola Company, DFI Retail Group, Grupo Éxito, Kerry Group, Kirin Holdings, Musgrave Group, Procter & Gamble, and Woolworths Holdings [128]. As such, their incorporation within the developed framework will significantly and unarguably augment efficacy.

The first factor, partnering for success, presents significant challenges for FMCGs. As the last value chain actor prior to the retailer or distributor, many feedstock suppliers and routes are available for partnerships or purchase agreements. Well considered selection of these suppliers and routes is critical in minimising negative impacts (be those environmental, economic, or social) over the full value chain. With these plentiful choices comes analysis problems, mainly in terms of permutation count. Considering a hypothetical process in which various feedstocks are combined to produce a consumer good, the number or possible supplier permutations increases rapidly. Figure 4-1, where data series one through six represent the number of different input materials required, shows a rapid increase in possible value chain permutations with both supplier options per feedstock material and number of feedstock materials required (note use of log scale on y-axis due to swift divergence). Consequently, limitations are placed on the assessment framework's structure. It must be capable of efficiently and comprehensively computing results for vast numbers of value chain permutations, without also increasing practitioner workloads relative to traditional assessments.

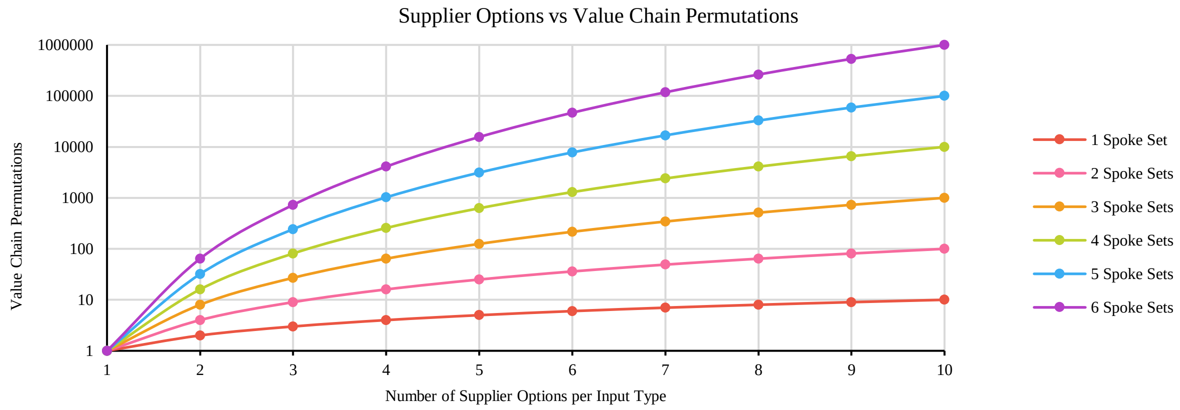

Figure 4-1 – Number of value chain permutations present as the number of spoke sets and constituent alternatives increases.

The second point identified by CGF and EY highlights the dependency on quantitative data to measure and track sustainability performance; a fact already identified during the definition of the chapter's guiding philosophy. With today's complex and geographically dispersed value chains, the effective identification, collection, and utilisation of impact pathway data is an emerging and growing challenge across all three assessment strands; however, it affects SIA disproportionately strongly. Development and adoption of such quantified SIA impact indicators in parallel to those already realised for LCA and TEA represents the last step in the dismissal of qualitative and subjective scoring, delivering significant value addition to FMCGs. As Identified in Chapter 3, prior to this research the quantification of social impacts through characterisation models represented a significant gap in capability, presenting a notable Achilles heel within not only FMCG oriented studies, but the field of sustainability assessment in general.

What constitutes the embedding of sustainability into the company DNA is subject to opinion. However, what is clear is the value of, and requirement for, the alignment of corporate strategy and sustainable development. With the attainment of quantitative impact characterisation across all strands, the benefits of which were outlined earlier, an ideal opportunity is presented for the application for multi-criteria decision analysis (MCDM). While numerous competing approaches exist (examined later), its incorporation facilitates the ranking of assessed systems, or value chains, based on impact indicator results and weightings. These weightings are tailored in alignment with the organisations broader strategy or external pressures and used to aggregate impact indicator results into an overall score through which alternatives can be ranked. Although introducing subjectivity through the weighting procedure, careful integration offers a useful tool to support both corporate steering and decision-making efforts.

Application of MCDM also offers benefits in terms of the CGF and EY report's fourth point, engagement, and communication with consumers. As a key stakeholder of FMCG companies, consumer opinions can influence the economic forecast of even the largest players [128]. Distillation of sustainability metrics to a single score may offer a clear and concise labelling and communication strategy, showcasing action and progress to the end-user. While deployment of these metrics to consumers is likely to fall under legislative purview of authorities, as observed with the EU's Ecolabel scheme [129] and ISO 14024 [130], it provides an enticing opportunity if compliance can be achieved.

Additional considerations, beyond those recognised by the CFG and EY report present themselves when considering the operability of assessment strands. For example, while large, the typical FMCG company has little influence or detailed process data beyond one or two up-stream value chain steps due to the commercial sensitivity. This limits their control over distant feedstock and supplier selection, while also resulting in opaquer LCI data. Consequently, any FMCG value-chain oriented assessment framework must not rely on attaining primary data, particularly beyond direct partners. Instead, extended value chain data must be approximated where necessary, based on relevant average technology performance; an approach mirrored within the widely utilised Ecoinvent database [131].

Following on from this, and the fifth point within the CGF and EY report, the assessment architecture should focus on the point at which the FMCG wields the most influence. Typically, this is either an in-house process, or a primary supplier's (who are often strategic partners [132]) process, where the options for change are much sparser. Beyond this pocket of high influence, FMCG's must select from an often-extensive pool of secondary supplier options and production routes. Common economic indicators, such as a plant's CapEx, is of little importance to FMCG companies beyond their sphere of influence; the more relevant true cost experienced is based on total OpEx of the upstream value chain and market conditions. This, therefore, requires a more nuanced consideration of some economic indicator's assessment boundaries.

Consequently, within this assessment framework CapEx will include investment requirements for process plant(s) under the FMCG companies' direct ownership or control (i.e. a maximum of one degree of separation), omitting capital considerations in the up- and down-stream value chain components considered within other indicators. Similarly, the OpEx of assessed value chains is also evaluated from the view of the FMCG company, yielding an "experienced OpEx" specific to their value chain step. This focusses on 'classical' OpEx contributions from the process plant(s) under the FMCG companies' direct control, incorporating factors such as maintenance, consumables, and external service provisions. However, unlike CapEx, the OpEx indicators must also include the purchase cost of feedstocks and energy utilised by the FMCG company's process step. Through this approach both OpEx and CapEx values of the value chain are calculated from the FMCG company's perspective. In essence, upstream and downstream CapEx requirements taken on by other organisations are reflected in the framework's OpEx indicator via feedstock purchase prices.

Finally, FMCG value chains typically operate at large scales and throughputs. Consequently, low TRL processes are highly unlikely to be pursued for deployment until risk can be mitigated through a proof-of-concept at pilot scale. This simplifies framework development as the many difficulties, such as the prediction of performance optimisation and lack of data associated with low TRL assessments, can be circumnavigated [39] [133]. With this in mind, the development of the framework can be optimised to best handle the assessment of processes residing at TRL 8-9.

4.5 Framework Architecture Development

To ensure the efficacy of the developed framework, several options for the structure and underpinning mechanics must be examined for suitability. This primarily focusses on the network topology used for the data exchanges, aggregation of the various value chain constituents, integration of MCDM, and LCI data formats and requirements. This section aims to outline and justify the methodological decisions that informed the final specification of the framework.

4.5.1 Network Topology Selection

The structure of the assessment, and its underpinning strategy, is analogous to network topology problems encountered within computer and systems engineering. Network topology refers to the process of systematically organising, arranging, or connecting several devices, in this case LCI datasets, in a network [134]. Considering the requirements for framework utility in the setting of FMCG companies discussed previously, several key criteria are outlined for the selection of the most applicable network topology strategy (see Table 4-2). Literature was consulted to determine which criteria are met by each strategy [134] [135] [136].

Table 4-2 – Attainment of desired attributes by alternative network topology structures [134] [135] [136].

Network Topology Strategy	Topology Selection Criteria			
	Focussed on a Core Node	Ability for Core Node to Specify and Scale Inputs	Direct Handling of Interchangeable Alternatives	Ability to Add or Remove Nodes
Hub & Spoke / Star	✓	✓	✓	✓
Ring				✓
Bus				✓
Tree	✓	✓		✓
Mesh				✓

As shown by Table 4-2, the hub and spoke (also commonly referred to as star) strategy is the only option that fulfils all specified criteria. While the tree strategy meets three of the four criteria, it is better suited to applications involving long chains of bifurcating nodes rather that direct interaction with a core node. Moving forward with the hub and spoke network topology (displayed in Figure 4-2), each of the core process', or hub's, feedstock types can be represented by a unique spoke interface. Each spoke interface acts as a lock and key mechanism, comparable to that observed in models of enzyme substrate complexes, allowing only spokes producing the correct material (or service) at the specified quality to interact (this can be viewed as a hub's elementary flow or, alternatively, a spoke set's reference flow). Groups of alternative spokes servicing the same interface are coalesced into 'spoke sets'. Individual spokes, therefore, form inventory modules that can be added, swapped, or repurposed in other assessments as desired.

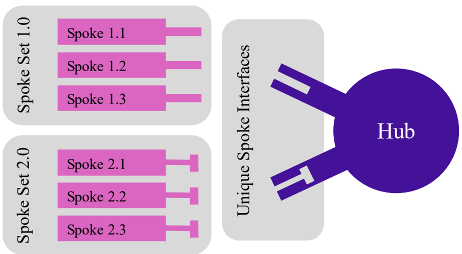

Figure 4-2 – Schematic to show the 'lock and key' approach to hub and spoke interfaces.

By assigning each spoke its own LCI, each set can be utilised in abstraction as a secondary comparative assessment of the locally available alternatives. This, in essence, acts as a miniature screening assessment, allowing FMCGs to reject poorly performing options at an early stage. Additionally, as a consequence of their conformation to the elementary flow specification of the hub process, spokes within a set deliver a perfect oranges to oranges comparison (harmonised spoke set reference flow), an achievement recognised in existing literature as challenging

[45]. In theory, there is no limit to the number of hub-spoke interfaces per hub, it is dependent only on the number of unique material or utility exchanges required by the process it represents. Similarly, there is no upper bound on the number of spokes that can reside within each set; however, as shown by Figure 4-1 the number of possible permutations will rise rapidly with set size.

4.5.2 Selection of Appropriate Multi Criteria Decision Making Technique(s)

Multi Criteria Decision Making (MCDM) is a historically rich field, with the first recorded example dating to c. 1011-931 BC and the biblical story of the 'Judgement of Solomon' [137]. In its more modern analytical sense, MCDM is employed to aid stakeholders in structuring decision making problems, identifying their preferences, and formulating aligned recommendations [138]. Prior to the rapid methodological developments of the 1960's, industry had used simple additive methods for the evaluation of competing 'alternatives', the theory of which was not greatly understood [139].

CDU as a field is, by definition, attempting to utilise carbon dioxide, combatting the still growing atmospheric concentrations (423.6 ppm average in the first half of 2024 [140]) while generating useful products. Ambitious climate targets such as the Paris Agreement [26] require that the allocation of capital and R&D efforts must be effective. Such complex problems necessitate the careful handling of trade-offs and non-uniform performance metric weightings. With finite capital and time available in the pursuit of climate targets such as the Paris Agreement [26], potential value chain components must be vetted, and their viability confirmed. This FMCG and CDU oriented application effectively utilises the strengths of MCDM, handling complex trade-offs and multiple stakeholders [141] [142] [143] [144].

Without analytical approaches, decision makers would primarily rely on 'gut feel' or similarly unsophisticated methods. Furthermore, despite introducing subjective value choices, the mathematical nature of MCDM provides a repeatable and justifiable decision-making process; 'quietening the noise' generated by criteria that are either unimportant, or potentially rectifiable at a later stage. Previous literature reviews have highlighted the increasing use of MCDM within environmental subject areas, growing four-fold from ~0.2% to ~0.8% of the field's publications between 2000 and 2015 alone [141].

Additionally, MCDM can greatly enhance the communicability of sustainability assessment results to non-practitioners. Results are often complex to interpret, delivering many indicator scores with incongruent units. While this granularity and specificity is invaluable to practitioners, how can they be effectively presented to the public or policy makers? A stakeholder with no LCA or sustainability assessment expertise can more meaningfully interpret results when presented through MCDM, often allowing for the comparison of alternatives in terms of a single score, incorporating all assessed criteria. With policy makers wielding significant influence over the pace at which climate mitigation proceeds, such a communication tool should not be undervalued.

Two fundamentally different approaches to MCDM have been precipitated; Multi Objective Decision Making (MODM) and Multi Attribute Decision Making (MADM) [145] [146] [147]. MADM methods incorporate four main components: alternatives, criteria, the relative importance of each criterion, and measure of performance of an alternative relative to a particular criterion [148]. These approaches target problems that contain a finite set of possible alternatives. Conversely, MODM approaches are suitable when evaluating undefined, or continuous, alternatives; it requires users to characterise constraints in the form of vectors reflecting decision variables [149]. Within CDU applications, alternatives represent processes or supply chain structures; consequently, they are finite in number and discretely defined, necessitating the use of MADM approaches. Due to its general inapplicability to the CDU field, MODM will not be considered further within this work. While many MADM methodologies employ complex mathematical principles, the overall process can be summarised by Figure 4-3.

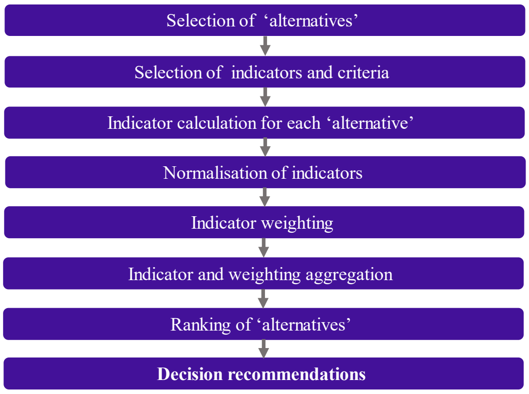

Figure 4-3 - Flow diagram of a typical MADM application (adapted from [150])

4.5.2.1 Multi Criteria Decision Making in Literature

A literature review of MADM within sustainability assessments focusing on CO_2 and CDU was conducted, aiming to examine current practices and methodological preferences. Web of Science was selected as the bibliographical database for use. Searches filtered for publication dates between 2015 – 2022, as well as identified keywords. Figure 4-4 shows the keywords used for each of the four rounds of searching, and the classification of each identified publication. A total of 72 publications were obtained, of which 44 are excluded (for reasons noted in Figure 4-4). The following analysis focusses on the approaches most frequently utilised; for this reason, review papers and novel methodological proposals are excluded. Duplicates and papers with no named methodology are also removed from the process. Finally, relevance of scope is used to exclude those that do not focus on carbon management, CDU, or sustainability assessment. This reveals 28 publications for examination (a table of the literature search results can be found in Appendix A).

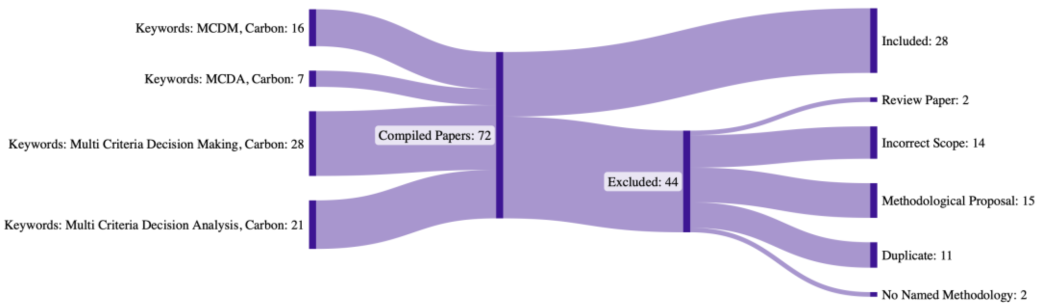

Figure 4-4 - Sankey diagram showing the quantity and usage of publications returned by the systematic literature search.

Methodologies employed by the included papers were then analysed, tabulating the frequency of use. A small number of papers used hybridised approaches, using part but not all of two or more methods without further modification. In these cases, each of the incorporated methodologies are given credit for usage. The results are shown by Figure 4-5, with methodologies including; data envelope analysis (DEA) [151], quality function deployment (QFD) [152], weighted sum model (WSM) (introduced by Fishburn and MacCrimmon [139]), evaluation based on distance from average Solution (EDAS) [153], stepwise weight assessment ratio analysis (SWARA) [154], complex proportional assessment (COPRAS) [155], decision making trial and evaluation laboratory (DEMATEL) [156], analytic network process (ANP) [157], élimination et choix traduisant la realité (ELECTRE) [158], preference ranking organization method for enrichment of evaluations (PROMETHEE) [159], viekriterijumsko kompromisno rangiranje (VIKOR) [160], analytic hierarchy process (AHP) [161], and technique for order of preference by similarity to ideal solution (TOPSIS) [162]. To allow for meaningful analysis and comparisons of methodologies, only those with more than one application case will be examined further, representing 83% of included publications.

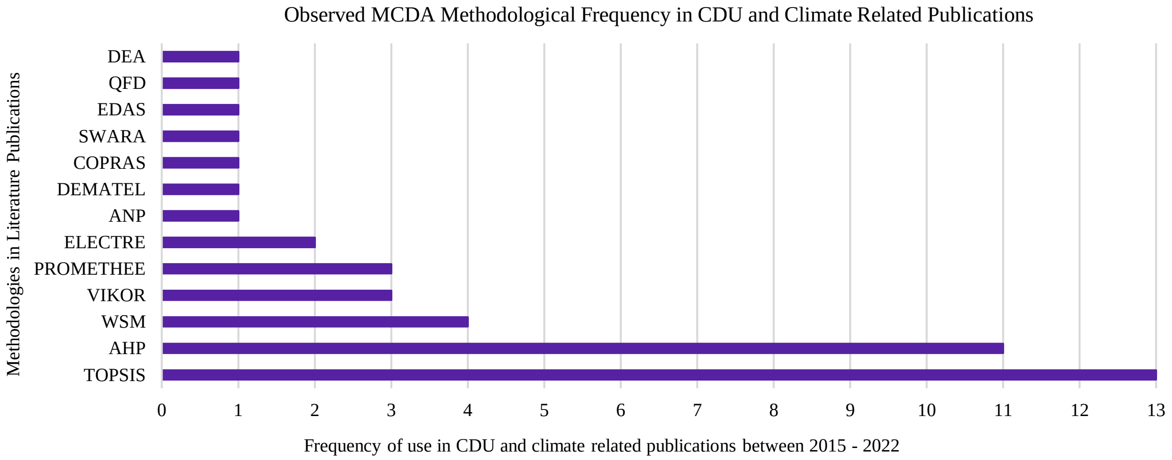

Figure 4-5 - Graph to show the frequency in which MCDM methodologies were observed through literature search

AHP and TOPSIS are the clear workhorses of CDU related MADM applications, appearing in 55.8% of publications and approximately three times more frequently than the third most common method. When the distribution in Figure 4-5 is compared to that in Figure 4-6, given by Sabaei, *et al*. in 2015, differences are observed. It should be noted that Sabaei examined MADM more broadly, choosing not to focus on applications within a specific field. However, this allows for comparison between general and CDU related applications. AHP is a frequent choice in both cases, whereas TOPSIS descends from most common in CDU related work to the least common generally, suggesting possession of characteristics advantageous within the methodologically nuanced field. Each examined method presents characteristic advantages and disadvantages, supporting rejection of a 'one size fits all' MADM approach. General principles, advantages, and disadvantages of each are discussed briefly before comparisons are drawn (full table of advantages and disadvantages is presented in Appendix A).

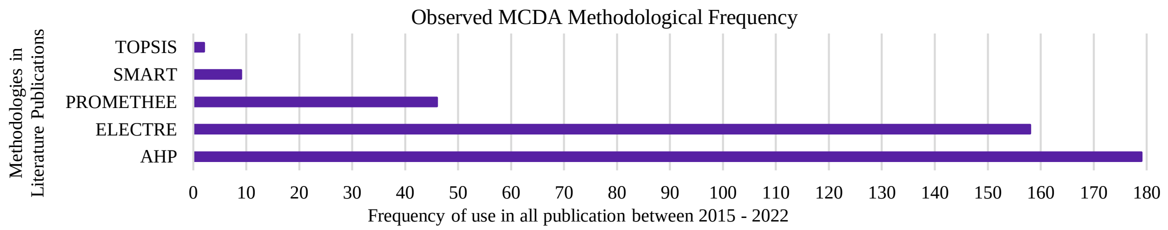

Figure 4-6 - Number of publications for various MADM techniques [163]

TOPSIS finds ideal solution based on the closest Euclidian distance to the positive ideal and farthest distance from the negative ideal. However, the relative importance of these distances is not considered through weighting [164] [160]. It is capable of handling very large numbers of alternatives with high computational efficiency while possessing a clear and intuitive logic [165]. However, the issue of rank reversal is present [166]; occurring when a change in rank ordering of alternatives is experienced in response to another being added to, or removed from, the evaluated set [167].

AHP focusses primarily on hierarchical problems [163], using decision maker value choices to mathematically determine criteria weights through matrices. Through this it allows for finer control and monitoring of decision-making consistency [168] [169], while facilitating group decision making [170] [171]. Due partially to this capability, it is suited to the allocation of resources and business effort [172], problems in which many stakeholders are usually present. Furthermore, it is appropriate for the integration of qualitative data [163] [173] using practitioner derived scoring scales. While weighting derivation is a characteristic strength of AHP, it can have significant influence on final scores or recommendations [174], potential mitigation strategies are explored in literature [175] [176]. Large criteria counts can also cause issues within AHP, affecting both workloads and consistency. AHP includes the calculation of a consistency ratio, quantifying how aligned successive practitioner inputs are; as the number of criteria, and therefore pairwise comparisons increase, it is harder to keep the consistency ratio within the acceptable range (prescribed by Saaty [177]).

The fastest of the MADM approaches, WSM, takes a highly transparent approach to score calculation; simply summing the product of criteria values and weights for each alternative. However, this simplicity results in several limitations. One of the most impactful is a failure to define interrelations between criteria [178]; reducing the techniques efficacy in complex decision-making contexts in which the balancing of conflicts is often necessary. Beyond this, such straightforward aggregation can lead to identical objective vectors for significantly different criteria weightings [179], limiting the granularity of possible insights. Additionally, small variations in weightings often cause a change in the recommended alternative, usually requiring a compensatory sensitivity analysis.

VIKOR handles large numbers of alternatives, a desirable quality in this application. Beyond this, the methodology is conceptually intuitive [180]. However, the procedure often results in erroneous alternative rankings due to flawed calculation methods for the maximum group utility and the minimum individual regret of the opponent, two of its primary calculation metrics [181]. Another shortcoming is revealed in criteria weighting determination, requiring hybridisation with other techniques for accurate and stable results [182].

PROMETHEE is characterised by the expression of user preference functions, used to generate a partial (PROMETHEE I) or full ranking (PROMETHEE II) of alternatives [183]. Requiring few user inputs compared to other prominent methodologies [184], PROMETHEE reduces workloads and potential for bias. There is also no requirement for normalisation of alternatives’ criteria scores [163], this step being included within the base methodology. Despite these advantages, the approach often exhibits loss of data or resolution if used to generate complete rankings [184], reducing the utility of any outputs. PROMETHEE also suffers from rank reversal phenomena [185], a trait shared with TOPSIS.

Finally, the ELECTRE family comprises of seven sub-methodologies are present (ELECTRE I, ELECTRE Iv, ELECTRE IS, ELECTRE II, ELECTRE III, ELECTRE IV, ELECTRE TRI) [186] [187], tailoring the approach to different problem types. ELECTRE I and ELECTRE III are the most applicable around CDU and sustainability assessment, tackling selection and ranking problems respectively. The methods allow for the prescription of 'veto' criteria, serving to remove undesirable alternatives [188]. However, resulting rankings depend on the size of this threshold, for which there exists no 'correct' value [163]. Literature also reports significant workload requirements [189], explaining the limited use seen in Figure 4-5.

4.5.2.2 Applicability Criteria

Key qualities associated with MADM selection have been identified, with Table 4-3 comparing the performance of examined methodologies against these attributes. References, along with further methodological advantages and disadvantages, can be found in Appendix A. All methodologies are seen to cater to a broad variety of scopes, while remaining applicable to cases containing large numbers of alternatives. Beyond this, the methodologies exhibit often significant divergences. As stated by others, there is no perfect MADM methodology, with selection required on a case-by-case basis [190]; the approach chosen can influence study outputs and introduce bias. Additionally, data availability influences the selection of methodology as explored by Sabaei, *et al*. [163].

Table 4-3 - MADM methodologies and associated attributes

Methodological Attributes	TOPSIS	AHP	WSM	VIKOR	PROMETHEE	ELECTRE
Directional Freedom of Scoring Scale	✓		✓	✓	✓	✓
High Number of Criteria	✓			✓	✓	✓
High Number of Alternatives	✓	✓	✓	✓	✓	✓
User Consistency Tracking		✓				
Broad Scope of Application	✓	✓	✓	✓	✓	✓
Weighting Generation Procedure		✓				
Aids Definition of Problem Structure		✓				

4.5.2.3 Technique Selection

Of the methodologies seen frequently in the literature search, only AHP includes a robust approach to weighting derivation. This represents a significant flaw in other methods as human perception and logic of prioritisation is prone to errors when more than four criteria are present [191]. Consequently, additional work is required to determine meaningful weightings, often involving hybridisation. Furthermore, through this integrated weighting procedure, AHP is the only method to track the consistency of user value-choices, safeguarding against conflicting inputs.

While AHP mathematically determines weightings, it is not suited to problems with large numbers of criteria; a consequence of its pair-wise comparison approach. In a comparison matrix with n criteria present, $\frac{n^2-n}{2}$ independent pairwise comparisons will be required. This sizable workload requires either a limited criteria count or more complex hierarchical structure, both effectively lowering the number of comparisons. Utilisation of the hierarchical approach also offers significant support in structuring complex problems including those seen in CDU sustainability assessments, a potential explanation for its widespread adoption. Both AHP and WSM also fail to handle problems with different criteria scoring directionality. This is facilitated in the other methodologies through matrix normalisation steps that account for either beneficial or non-beneficial criteria. While this is inconvenient in many contexts, the issue can be overcome through the addition of a normalisation step using either utility curves or linear scaling.

4.5.2.4 Implementation Within the Assessment Framework

As detailed previously, each MADM approach has specific advantages and disadvantages. When seeking the best method for a given field or problem type, these must be considered both in isolation and in hybridised forms. Hybridisation likely offers the best approach, retaining strengths while resolving weaknesses. Such approaches can be seen throughout literature with many different technique combinations [192]. The first appeared in 1999 [193], with the term Hybrid Multi Criteria Decision Making being coined by Shyur and Shih in 2006 [194].

To identify suitable methodologies, the requirements of the application must be defined. For use in CDU and FMCG oriented sustainability assessment, the following factors are determined as important:

- Systematic and repeatable criteria weighting procedure
- User value choice consistency checking to prevent conflicting preference prescription
- Transparency of calculations
- Applicability to problems with many criteria
- Satisfactory computational and workload efficiency

After identifying these requirements, the assessed methods can be examined for suitability, supported by Table 4-3. AHP and TOPSIS appear ideal for hybrid application; perhaps unsurprisingly given their combined 55.8% prevalence in the earlier systematic literature search. Arslan, *et al*. previously reviewed the hybridization of these two methodologies, determining that their integration produces a more powerful and effective decision-making tool [195]. This approach will now be examined further in the context of CDU sustainability assessment applications.

AHP, developed by Saaty [196], already appears within environmental decision making [197], consistently being noted as a common technique in the area [198] [199]. In addition, it is the only methodology that can fulfil the first two requirements laid out for this application: systematic and repeatable criteria weighting, and user value choice consistency checking. Furthermore, the approach's tiered hierarchical structure aligns well with the format of McCord, *et al*'s. triple helix framework [7]; alleviating the pairwise comparison workloads associated with high criteria counts. The number of pairwise comparisons required for both global and tiered AHP approaches can be derived Equation 4-1 and Equation 4-2 respectively. This is represented in a two-tier configuration by Figure 4-7 (analogous to the approach taken by Chauvy, *et al*. [197] for different applications). In addition, a hierarchical approach allows for application of a zero weighting to one or two entire strands (tier 1); therefore, excluding them and delivering a double or single stranded assessment.

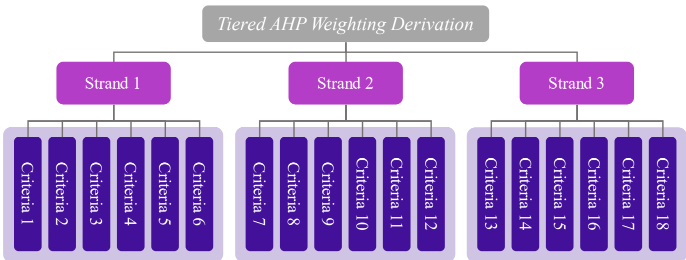

Figure 4-7 - Tiered AHP structure (based on that described by Chauvy, et al. [197]. S_i represent assessment strands.

Equation 4-1 - Calculation for the number of pairwise comparisons required for a global AHP approach. Where C is the number of criteria assessed.

$$\frac{C^2 - C}{2} = pairwise\ comparions\ (global)$$

Equation 4-2 - Calculation for the number of pairwise comparisons required for a tiered AHP approach. Where S is the number of strands employed, and C is the number of criteria assessed. (Assuming criteria are distributed evenly between strands)

$$S\left(\frac{\left(\frac{C}{S}\right)^2 - \left(\frac{C}{S}\right)}{2}\right) + \frac{S^2 - S}{2} = pairwise\ comaprisons\ (tiered)$$

If calculated across varying total criteria counts, the difference in pairwise comparisons and workload can be seen visually (Figure 4-8). As the number of criteria assessed increases, the required pairwise comparisons diverge; consequently, efficiency increases with assessment granularity. For example, studies evaluating 18 criteria experience a 68.63% reduction in practitioner workload when using a tiered approach. With many assessments needed to evaluate growing numbers of emerging CDU technologies, an efficient methodology will prove invaluable.

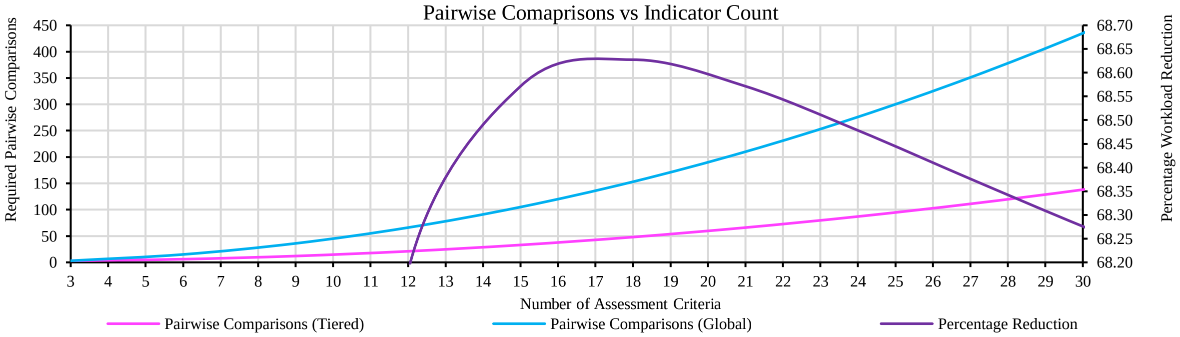

Figure 4-8 - Evaluation of pairwise comparisons required for the implementation of AHP in tiered and global structures and criteria count increases (based on application to the triple helix framework [7] with three AHP sub-tiers and an even indicator distribution). Percentage workload is overlaid using a secondary axis.

Due to the abundance of literature outlining the mathematical procedure for AHP weighting derivation, and its unaltered adoption for this sub-section of the framework's MCDM module, this will not be outlined in detail within this work. However, once criteria weights have been determined, the outputs can be fed directly into TOPSIS in order to generate a ranking order of the available alternatives. This hybridisation strategy eliminates the weaknesses of both methodologies; the aggregation, scoring scale directionality, and ranking within AHP, and the weighting derivation within TOPSIS. Furthermore, TOPSIS is capable of handling very large numbers of alternatives with high computational efficiency while possessing a clear and intuitive logic [165], facilitating more detailed assessments. This delivers a strong foundation for applications such as value chain selection, in which many structural permutations are present. However, the issue of rank reversal persists [166]. To combat this, sensitivity analysis is recommended to verify the stability of generated results as the weights vary.

When qualitative data is presented, such as that seen in most social impact assessments, a five or nine-point scale should be used for the assignment of quantitative values within the TOPSIS decision matrix. This is prescribed to achieve better differentiation between alternatives, as suggested by McCord *et al*. within the triple helix framework's SIA reference scale-based characterisation method [7]. Once the decision matrix is created, vector normalisation is carried out by criterion using Equation 6-3.

Equation 4-3 - Vector normalisation procedure for alternative criteria scores. Where, m is the number of alternatives examined, i is the specific alternative considered, and j is the specific indicator considered.

$$V_{ij} = \frac{X_{ij}}{\sqrt[2]{\sum_{i=1}^{m} X_{ij}^2}}$$

The standard TOPSIS methodology can then be applied as developed by Hwang and Yoon [162]. For each criterion the best and worst scores are identified, V_j^+ and V_j^- respectively. Using these, the Euclidian distance from best (S_i^+) and worst (S_i^-) performance values can be calculated for each alternative.

Equation 4-4 - Calculation of the Euclidean distance from the ideal best performance. Where, n is the number of criteria assessed, i is the specific alternative considered, and j is the specific indicator considered.

$$S_i^+ = \left[\sum_{j=1}^{n} \left(V_{ij} - V_j^+\right)^2\right]^{0.5}$$

Equation 4-5 - Calculation of the Euclidean distance from the ideal worst performance. Where, n is the number of criteria assessed, i is the specific alternative considered, and j is the specific indicator considered.

$$S_i^- = \left[\sum_{j=1}^{n} \left(V_{ij} - V_j^-\right)^2\right]^{0.5}$$

The overall performance score for each alternative, accounting for all criteria, can then be evaluated (P_i). This provides the basis on which the alternatives are ranked. Opricovic (developer of VIKOR) and Teng suggest that the efficacy of TOPSIS may be improved by allowing the user to weight the importance of the Euclidean distance from the deal best and worst scenarios [160]. This would allow for more problem specific application of both independent and hybridised TOPSIS. However, for a majority of problems, including CDU value chain assessments, the standard equal weighting approach is deemed satisfactory.

Equation 4-6 - Calculation of alternatives i's overall performance score (P)

$$P_i = \frac{S_i^-}{S_i^+ + S_i^-}$$

4.5.3 Data Architecture

With the network topography and MCDM strategies selected, and their suitability explored, the detailed architecture must be developed and examined through the practitioner's lens. To this end, the framework is approached in a compartmentalised fashion, examining the data flows through and between the following areas; impact characterisation approach, inter-module umbilical specification & data sheet development, lifecycle inventory generation & analysis, spoke set normalisation & performance matrix generation, decision maker's indicator weighting calculation, ranking & selection of value chain permutations, and aggregation of hub & spoke modules. These are discussed in sequence and interface to produce the architecture shown by the data-oriented flow sheet in Figure 4-9. The overall model is presented first to aid communication of the following section.

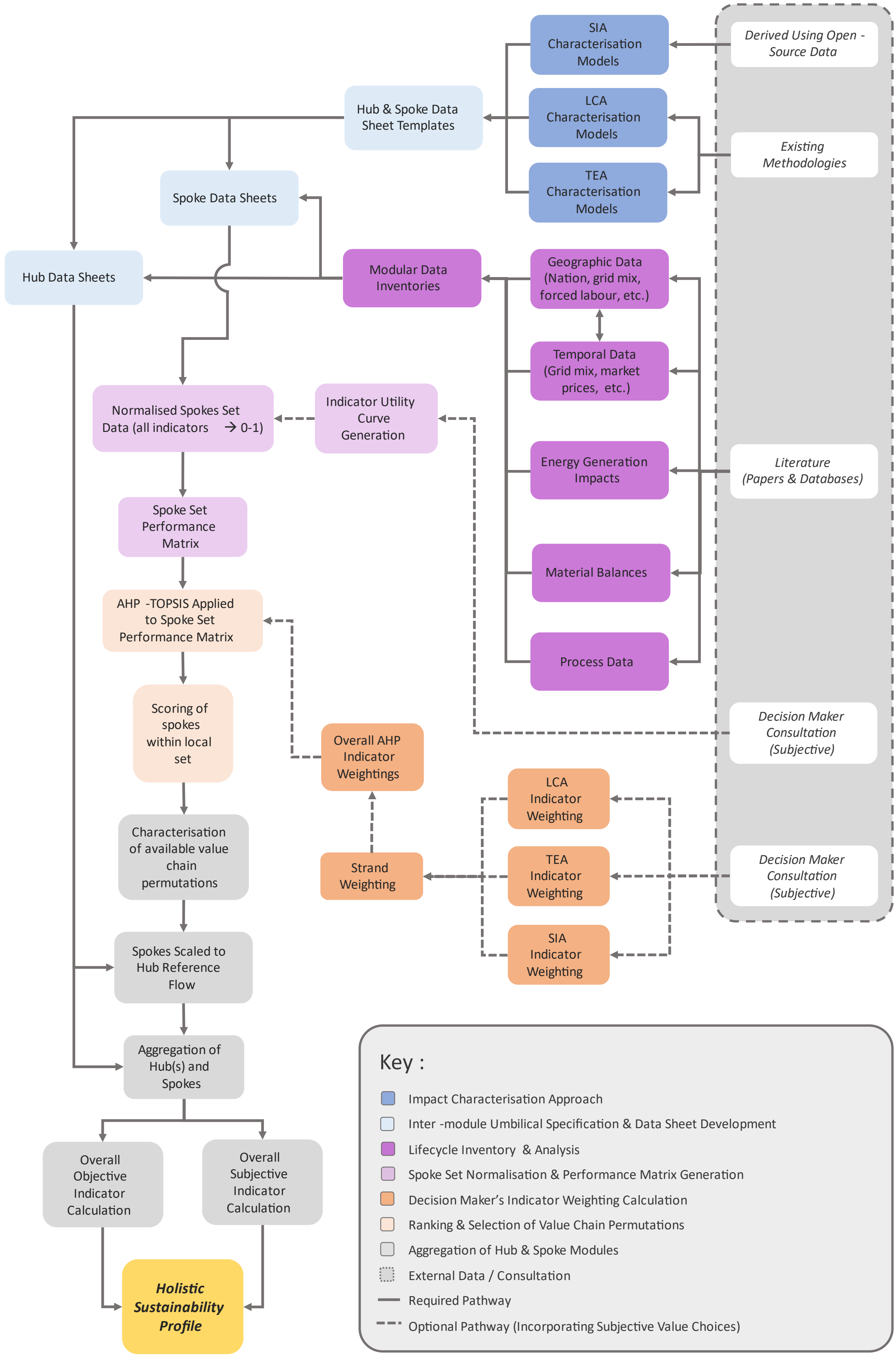

Figure 4-9 – Schematic of the developed framework's data architecture.

4.5.3.1 Impact Characterisation Approach

Despite the selection of impact indicators on a case-by-case basis, their accurate quantification through repeatable and objective characterisation methods are a keystone of well executed LCAs. While TEA offers some degree of standardisation with respect to characterisation procedures, the social strand lags behind significantly [19]. As a result, the framework's LCA and TEA strands utilise pre-existing, recognised characterisation methods. Many competing alternatives are available, the selection of which is left to the practitioner's discretion as observed in other assessment standards [55], guidelines [39] and frameworks [7]. However, the employed approach should be widely recognised and internationally accepted, ensuring the usability and validity of the generated results.

The social strand introduces a significant challenge with respect to the characterisation of impacts. Due to its relative youth as a field [200], impact pathway models comparable to those used in LCA are yet to be developed. In their place, practitioners are currently advised to use a reference scale approach [7] [201] [202], these detail indicator specific criteria against which practitioners score assessed systems. Discrete five- or nine-point scales are typically used, as noted by McCord, *et al*. [7], significantly limiting the achievable resolution. Furthermore, this reliance upon practitioner judgement unavoidably adds subjectivity to the process, preventing full harmonisation with the LCA and TEA strands. Consequently, the development of initial quantified, impact pathway based, social impact characterisation models is deemed necessary in order to deliver a fully harmonised and holistic assessment framework.

In the pursuit of quantified and repeatable social impact characterisation, several facts must be recognised. Firstly, the development of characterisation models in LCA was a time intensive process, requiring iteration and refinement of the respective methodologies. In addition to this, the impact pathway is significantly more complex. Where environmental impact pathways remain constant with changing geography and cultures, social impact pathways can vary, potentially greatly; different cultures and demographics will respond to societal changes in unique ways. As a result, measuring and characterising these response mechanisms systematically is a monumental challenge. To resolve these issues around complexity and accuracy, it is decided that the social strand should function as a national level red-flag assessment, highlighting areas of the value chain in which increased risk is likely to be observed. Consequently, the impact characterisation models should be referred to as 'red flag' in the interest of transparency as they do not measure definite impacts, but rather identify areas of elevated risk where adverse social outcomes are more likely based on universally applicable contributing factors. By using this approach in conjunction with national-level data, the framework functions as a broad, social risk screening tool. This facilitates the flagging of countries that may require elevated due diligence, scrutiny or mitigation strategies with respect to a given indicator during a projects planning or deployment phases. A full elucidation of the development and evaluation of each of developed social characterisation models is given in Chapter 5.

To maintain alignment with practices seen in LCA and TEA impact characterisation, open-source data is to be used for the social strand. While this succeeds in delivering transparency, a pivotal aspect of sustainability assessment, compromises must be made in terms of resolution. For the purposes of the framework, a national level assessment is deemed sufficient to identify potential social issues and indicate a requirement for increased due diligence and care. Reporting of each strands impact indicators should be approached in terms of the local (either spoke’s or hub’s) functional unit. This step aids with the later aggregation and dynamic scaling of impacts when considering intermediate flows of varying magnitudes.

4.5.3.2 Inter-Module Umbilical Specification & Data Sheets

Having previously selected the hub and spoke network topology (discussed in Section 4.5.1), the interface between the two module types must be standardised. For system and impact data to flow correctly throughout the model several pieces of information must be exchanged in each direction. A summary of these required data flows is given in Table 4-4. Only the minimum necessary information required for a complete assessment is exchanged to help maintain simplicity, modular integrity, and inter-operability. To resolve complex system related queries and maintain data quality, complimentary standardised data sheets are also developed to fully detail each hub and spoke modelled; this approach takes inspiration from the LCI datasets generated by Ecoinvent.

Table 4-4 – Details of data transfer and it’s directionality between hubs and spokes within the framework.

Hub to Spoke	Spoke to Hub
Material type and requirements (purity, phase, etc.)	Objective impact indicator results
Quantity required per FU	Spatial setting
	Temporal setting

The material types required by the hub process are specified at their respective interfaces, and fulfilled by the matching spoke, or set of spokes. At this point, any required conditions or purity constraints must be specified to ensure compatibility with the hub process. In less sensitive processes, an acceptable range may be specified. Flexibility is built into the framework’s methodology where possible to cater to the widest possible range of systems and assessment resolutions.

Hub’ are also the arbiters of the reference and intermediate flows upon which the value chains LCI is constructed. Each of the hub’s input and output flow LCIs should be evaluated on a local mass basis. This allows the spokes local impact indicator results to be scaled up or down to reflect the hub’s utilisation rate. For instance, a hypothetical set of spokes, detailing the production of ammonia at equitable quality, would each have a local functional unit of 1 tonne. For example, if a hub interface specifies a requirement of 1.8 tonnes per tonne of final product, the spokes’ impact objective indicator results must be multiplied by 1.8 to homologate the spoke and hub at the interface.

Spokes are primarily responsible for the provision of independent LCIs and impact indicator results for each feedstock option considered by the FMCG company. These spoke datasets should be detailed and organised such as to function as standalone assessments (typically with a cradle-to-gate scope). The objective impacts should be evaluated using consistent characterisation models such as ReCiPe or TRACI to ensure the fair comparison of the locally competing spoke set alternatives. In addition to this, the spokes should also contribute contextual information to the full assessment. Any assessment requires the definition of the overall system’s boundary, in which the organised and systematic communication of each spoke’s spatial and temporal relevance is key.

To ensure the consistent communication of the outlined information flows, a standardised data sheet is required. This must act as a full account of the spoke’s local assessment including the first three phases of ISO’s four phase format (goal and scope, lifecycle inventory, and inventory analysis) [55]. The fourth and final aspect prescribed by ISO, interpretation, is suspended in favour of execution over the whole value-chain, post-aggregation (as indicated by Figure 4-10). Blank templates for the hub and spoke datasheets are included in the supplementary material (Appendix B) for evaluation. Additional data beyond that specified in Table 4-4 is included within the data sheets, helping to capture each of the sub-assessments' respective details. This includes a system diagram, technology description, any assumptions employed (with justification), stream tables, and included unit operations. With the capture of this information, each hub or spoke within a larger assessment can be critically and transparently evaluated, checking for validity and completeness.

4.5.3.3 Lifecycle Inventory Generation & Analysis

While the hub and spoke's local LCIs and LCIAs are characterised within their respective data sheets, the larger assessments LCI/LCIA is structurally complex. To maintain a manageable volume of data flowing throughout the model, only the objective indicator results, in terms of the homologated spoke set's local functional unit, are added directly to the global LCI (shown by the schematic in Figure 4-10). This approach delivers a set of matrices covering the hub impacts and each spoke set independently (shown by Table 4-5). Such an intermediate step, examining each spoke set in isolation, is required for the integration of AHP-TOPSIS (discussed later).

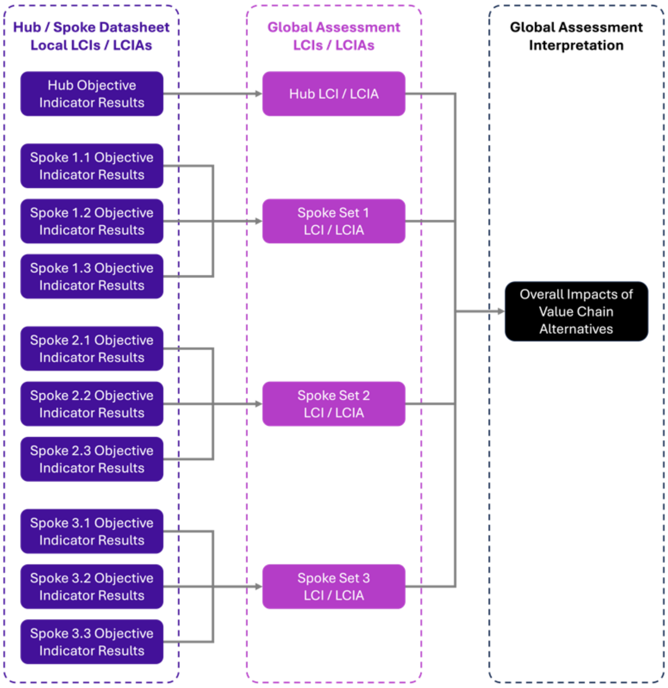

Figure 4-10 – Schematic to show data extraction flow between the standardised hub and spoke data sheets, assessment LCI, and interpretation phase.

Table 4-5 – Format of spoke set performance matrix containing objective indicator results for all constituent alternatives.

	Spoke Set Constituents - Objective Indicator Results		
Indicator	1.1	1.2	1.3
a	$I_{1.1,a}$	$I_{1.2,a}$	$I_{1.3,a}$
b	$I_{1.1,b}$	$I_{1.2,b}$	$I_{1.3,b}$
c	$I_{1.1,c}$	$I_{1.2,c}$	$I_{1.3,c}$
d	$I_{1.1,d}$	$I_{1.2,d}$	$I_{1.3,d}$
e	$I_{1.1,e}$	$I_{1.2,e}$	$I_{1.3,e}$

As indicated by Figure 4-10, the assessment LCIs / LCIAs converge further with each data handling step. This does, however, add limitations to the constituent assessments. Probably the most obvious is the requirement that indicators be assessed uniformly over all spoke sets. Such uniformity does not simply apply to the indicator selection, but also the characterisation models utilised. Restrictions such as these offer potential constraints around the inter-operability of assessment modules, an underpinning concept within the framework. However, it is expected that a FMCG company of a size that requires complex value chain assessments is aware of what indicators it deems important with respect to impacts and decision making. Therefore, the indicators should be consistent across all in-house assessments, nullifying the harmonisation issue. A single exception to the requirement for indicator alignment is observed, specifically the consideration of CapEx. As discussed in the guiding philosophy, CapEx is only pertinent to the processes under the FMCG's direct control (the hub), with spokes only aiming to characterise the realised purchase price of services or feedstocks.

The isolated consideration of spoke sets thus far adds flexibility to the assessment's application. System boundaries can be tailored around each spoke set individually while still maintaining comparability between value chain permutations. For instance, an FMCG company may require spoke set one to assess its feedstock on a cradle-to-gate basis, while spoke set two uses a gate-to-gate boundary. An option must be selected for each spoke in every possible value chain permutation, maintenaning of a consistent overall boundary. However, this bespoke approach comes at a cost, departing from the commonly recognised assessment boundary configurations.

4.5.3.4 Spoke Set Normalisation & Performance Matrix Generation

With the objective LCI and LCIA data for each spoke set aggregated in the format of Table 4-5, a secondary data stream evaluating the relative utility to a FMCG company can be generated, forming the a basis for application of the AHP-TOPSIS MCDM module. This parallel stream is built upon the local normalisation of the spokes' objective indicator values. However, as identified by McCord, *et al*. within the triple helix, care must be taken to ensure correct and harmonised scoring directionality. That is, should beneficial or detrimental scores be assigned higher values? It is recommended that within the framework high scores should indicate a positive performance, appealing to intuition and enhancing interpretability.

In some specific cases, greater insight may be extracted by specifying a utility curve for the normalisation of results, facilitating the consideration of non-linearity or prescribed upper/lower constraints (as observed later in Chapter 5, Section 5.5.3 during the characterisation of the social strand's 'Risk of Change in Access to Electricity' indicator). When applying utility curve-oriented normalisation, it is important that practitioners be vigilant of the potential for the introduction of bias; this can typically be examined through a sensitivity analysis. Generally, a linear max-zero or max-min based normalisation is suggested.

The local normalisation of spoke sets sequentially considers each of the indicators, and the associated range of performance over the available alternatives. When the objective is minimisation of the indicators value, as is the case for GWP, Equation 4-7 is used, simultaneously normalising between zero and one, while correctively reversing directionality. Contrasting this, indicators such as energy efficiency target maximisation, requiring the application of Equation 4-8; in these cases, the normalisation process is simpler as scoring directionality does not need to be reversed. The results are compiled in a secondary, normalised, iteration of Table 4-5 (shown by Table 4-6).

Equation 4-7 – Normalisation procedure for indicators in which low objective values are preferable. Where I_{ij} is the objective performance of alternative j in terms of indicator i, and $\hat{I}_{ij}$ is the normalised performance of alternative j in terms of indicator i.

$$\hat{I}_{ij} = 1 - \frac{I_{ij}}{I_{j_{MAX}}}$$

Equation 4-8 - Normalisation procedure for indicators in which high objective values are preferable. Where I_{ij} is the objective performance of alternative j in terms of indicator i, and $\hat{I}_{ij}$ is the normalised performance of alternative j in terms of indicator i.

$$\hat{I}_{ij} = \frac{I_{ij}}{I_{j_{MAX}}}$$

Table 4-6 – Format of normalised indicator results matrix for a given spoke set.

	Spoke Set Constituents - Normalised Indicator Results		
Indicator	1.1	1.2	1.3
a	$\hat{I}_{1.1,a}$	$\hat{I}_{1.2,a}$	$\hat{I}_{1.3,a}$
b	$\hat{I}_{1.1,b}$	$\hat{I}_{1.2,b}$	$\hat{I}_{1.3,b}$
c	$\hat{I}_{1.1,c}$	$\hat{I}_{1.2,c}$	$\hat{I}_{1.3,c}$
d	$\hat{I}_{1.1,d}$	$\hat{I}_{1.2,d}$	$\hat{I}_{1.3,d}$
e	$\hat{I}_{1.1,e}$	$\hat{I}_{1.2,e}$	$\hat{I}_{1.3,e}$

It is important to note these two equations result in normalised values that are dependent on the observed impacts across the spoke options. In the event that all perform similarly, the normalisation procedure should be re-evaluated by the practitioner, considering instead the use of independent upper and lower bounds. In such spoke sets, containing indicator results clustered tightly about a low maximum observed value, differentials in performance will be magnified. As an example, consider two spoke sets, each with three alternatives. Their respective hypothetical GWP objective indicator results, and associated normalised values, are given in Table 4-7. As can be seen in the normalised results (calculated using Equation 4-7), the tight clustering and small magnitude of the highest observed objective GWP value in set 2 culminates in misleading normalised outputs. In most ordinary cases this methodological artifact is advantageous, delivering normalised results relative to the options available to the FMCG company. However, in this very specific case, a more representative assessment may be realised through the introduction of an artificial $I_{j_{MAX}}$, or benchmark spoke, ensuring the presence of a representative upper bound and meaningful normalisation. Alternatively, utility curves can be employed to remove these issues, potentially also introducing utility limits above or below which scores of one or zero are assigned uniformly. For example, a utility curve for GWP may exhibit a hard limit of 1,000 kg CO_2-Eq. per FU, above which a normalised indicator score of zero is prescribed to prevent a 'range runaway' and its associated detrimental effects on the indicator normalisation and subsequent local spoke rankings.

Table 4-7 – Example table showing hypothetical GWP objective indicator results for 3 alternative spokes and corresponding normalised results.

Spoke Options	GWP Objective Indicator Results (kg CO_2-Eq / FU)		GWP Normalised Results	
	Spoke Set 1	Spoke Set 2	Spoke Set 1	Spoke Set 2
Alternative 1	10	2	0.8947	0.7778
Alternative 2	40	6	0.5789	0.3333
Alternative 3	95	9	0	0

After the conclusion of the normalisation procedure the second results stream can be considered established, delivering a table mirroring the appearance of Table 4-6 but instead containing normalised values with harmonised directionality. The original objective results are ringfenced at this point, ensuring that robust and quantified assessment results are available in parallel to the subjective scores, the derivation procedure of which is detailed from this point onwards.

4.5.3.5 Decision Maker's Indicator Weighting Calculation

In the preceding evaluation of relevant MCDM techniques, hybridised AHP-TOPSIS was identified as the most appropriate technique for a FMCG value-chain oriented assessment framework (Section 4.5.2). The challenge in this application case is systematic and approachable integration alongside the objective results strands. Due to their application in series, AHP for weighting derivation followed by TOPSIS for ranking alternatives, each technique can be discussed in isolation.

The AHP section of the MCDM module is the only aspect that must be directly decision maker facing, requiring the pairwise comparison of assessed impact indicators. Following from the logic outlined in Section 4.5.2.4, a nine-point scale (shown by Table 4-8) is selected, delivering an appropriate degree of differentiation in assignable scores [7]. This scale is applied sequentially to the four sub-matrices (one inter-strand and three intra-strand) defined in the tiered structure identified in Figure 4-7, reducing decision maker workloads by up to 68.83% [203].

Table 4-8 – AHP scoring scale used within the hub and spoke framework

Scoring Scale	
Extremely Strongly Preferred	*9*
Very Strongly Preferred	*7*
Strongly Preferred	*5*
Moderately Preferred	*3*
Equally Preferred	*1*
Moderately Not Preferred	1/3
Strongly Not Preferred	1/5
Very Strongly Not Preferred	1/7
Extremely Not Preferred	1/9

To support effective use by non-practitioners, the four input tables should be incorporated within a data sheet clearly conveying their inter-relation. An example of such a data sheet, developed as part of the proof-of-concept study in Chapter 6, is shown in Figure 4-11. The hierarchical structure of the four input tables is shown in the top left, along with drop down menus allowing for the selection of weighting calculation options (listed and characterised in Table 4-9). The input matrices themselves are shown in the bottom half of the datasheet, and the resulting indicator weights in the top right. Pair wise comparisons are made in each 'cell' by consideration of the importance of the row indicator relative to the column indicator.

Table 4-9- Weighting methods available for inter- and intra-strand weighting calculation within the hub and spoke framework.

AHP Table	Calculation Approaches Available	Reason for Inclusion
Inter-Strand	Weighted by Indicator Count	Evenly distributes the strand weightings to account for their relative indicator counts. This delivers equitability to the strands and is the suggested choice for most applications.
	Decision Maker Value Choices	Allows for the subjective adjustment of strand weightings based on the FMCG's perceived importance.
	Uniform	Assigns a uniform weight of $0.\dot{3}$ to each strand.
Intra-Strand	Decision Maker Value Choices	Allows for the subjective adjustment of each strands' constituent indicator weightings based on the FMCG's perceived importance.
	Uniform	Assigns a uniform weight of n^{-1} to each indicator within the strand, where n is the number of constituent indicators present.

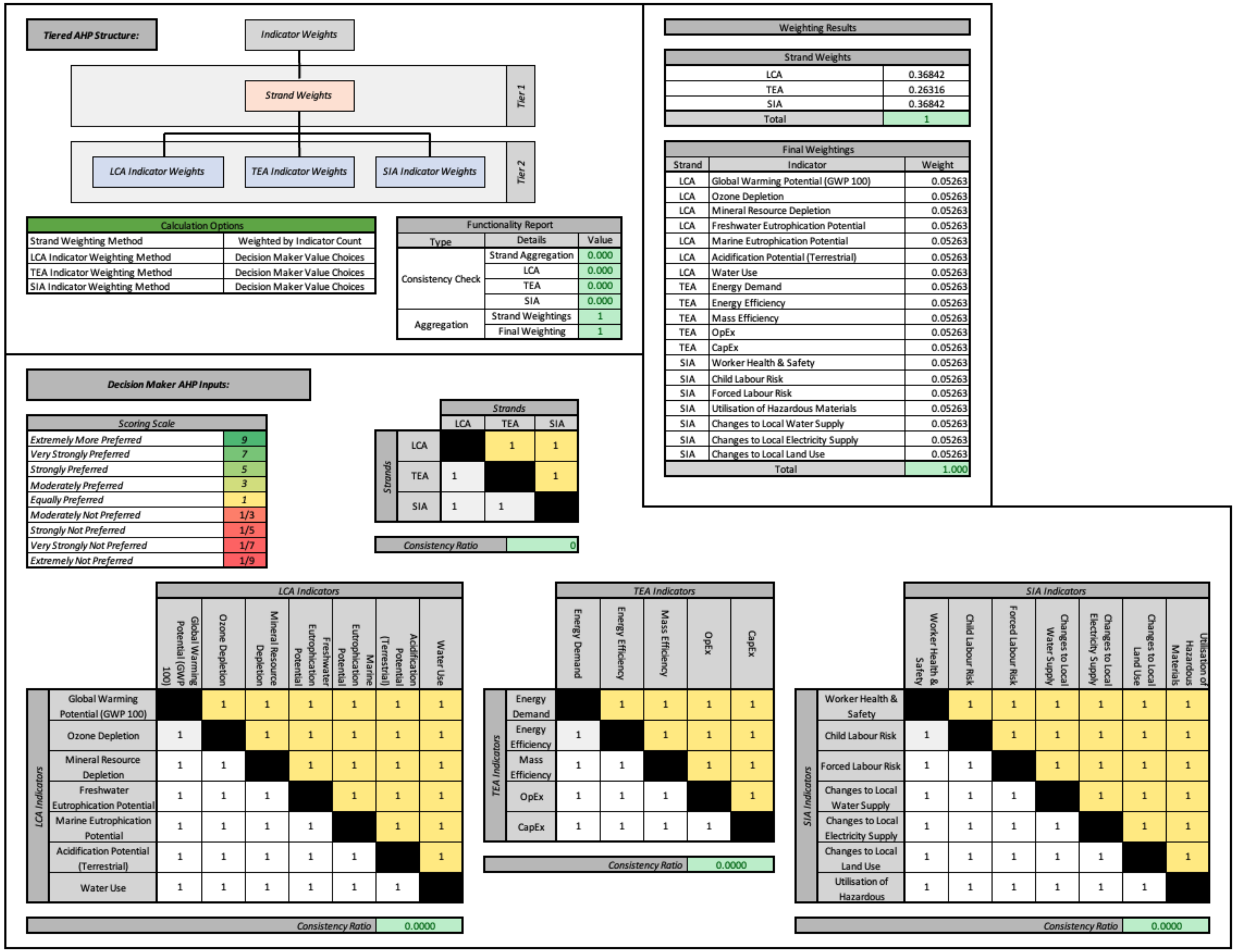

Figure 4-11 – User input pane for the hub and spoke model's AHP module. Top right shows method selection, top right shows final derived indicator and strand weights, bottom shows pairwise comparison matrices.

Another important consideration is the degree of consistency observed within the user's inputs, this can be quantified through the consistency ratio, prescribed by Saaty [177]. It's value must be less than 0.1 for the evaluated inputs to be valid [204]; however, there are exceptions for matrices of order three and four, having acceptance thresholds of 0.58 and 0.8 respectively [196]. If above the acceptable value, the user must re-evaluate and correct conflicting inputs until the threshold is met. Pant, *et al*. succinctly describe the typical scenario through which scoring inconsistencies arise [205];

> "*Assume that there are three criteria x_1, x_2, and x_3. The decision-maker finds that x_1 is slightly more important than x_2, while x_2 is slightly more important than x_3. If the decision-maker concludes, that x_3 is equally or more important than $x1$, then certainly some inconsistency arises. But, if the decision-maker concludes that x_1 is also slightly more important than x_3, then this decision is better than the earlier one and thus a slight inconsistency arises in this case. Hence, the second judgement is more consistent*."

Calculation of the Consistency Ratio (*C.R.*) for each matrix utilises the Consistency Index (*C.I.*), defined in Equation 4-9, where n is the number of assessment indicators present, and λ_{max} is the matrix's principle eigen value. A perfectly consistent matrix will deliver a $\lambda_{max} = n$ (realising a *C.I.* of zero), with inconsistent matrices λ_{max} being $\geq n$ (realising a *C.I.* > 0).

Equation 4-9 – Calculation of the consistency index (evaluating user inputs) within AHP's methodology. Where; λ_{max} is the matrix's principle eigen value, and n is the number of criteria present.

$$C.I. = \frac{\lambda_{max} - n}{n - 1}$$

This consistency index is then employed within Equation 4-10 to calculate the final Consistency Ratio. *R.I.*, the random consistency index is also specified by Saaty and is dependent on n (detailed in Table 4-10) [196]. The resulting consistency scores are displayed below each of the four matrices (see Figure 4-11), immediately making the user aware of any problematic inputs resulting in assessment validity issues.

Equation 4-10 – Calculation of the consistence ratio

$$C.R. = \frac{C.I.}{R.I.}$$

Table 4-10 – AHP random consistency indexes, adapted from Saaty, et al. [196]

n	3	4	5	6	7	8	9
R.I.	0.58	0.8	1.12	1.24	1.32	1.41	1.45

Once the local weightings are determined for each of the AHP matrices, the global weightings can be determined. The overall, or global, weighting of a given indicator is the product of its parent strand's assigned weight (Tier 1), and the indicator's local weight within its respective strand (Tier 2) (shown through Equation 4-11). This process ensures that the global sum of all indicator weights remains equal to one.

Equation 4-11 – Calculation of overall indicator weightings from the relevant tier 1 and tier 2 AHP weighting results.

$$Overall\ Indicator\ Weighting\ (W_j) = W_{Tier\ 1} \times W_{Tier\ 2}$$

4.5.3.6 TOPSIS Derived Spoke Ranking

With the global indicator weights defined through AHP, they must be combined with the normalised spoke indicator results from Section 4.5.3.4 prior to utilisation within the TOPSIS section of the MCDM module. To prepare the normalised spoke set data (as presented in Table 4-6) for use in a TOPSIS applicable matrix, the normalised indicator scores ($\hat{I}_{ij}$) are multiplied by their corresponding AHP derived weighting (W_j). This procedure is carried out set wise, delivering a matrix containing the criterion scores (V_{ij}) for each spoke (i) and indicator (j) pair.

Equation 4-12 – Calculation of criterion score (V_{ij}) for spoke i's indicator j performance from the normalised indicator score $\hat{I}_{ij}$ and AHP derived indicator weighting W_j.

$$V_{ij} = \hat{I}_{ij} \times W_j$$

The TOPSIS methodology is then applied to the normalised and weighted spoke set data, as outlined in Section 4.5.2.4 through Equation 4-4, Equation 4-5, and Equation 4-6. Thus, an overall score between zero and one is realised for each spoke option assessed; in which higher scores denote closer proximity to the ideal solution in n^{th} dimensional Euclidian space (where n is the number of indicators assessed). This score acts as a measure of the alignment of the spoke's impact profile with the FMCG company's AHP value choice inputs (relative to the available alternatives).

4.5.3.7 Aggregation of Hub & Spoke Modules

The comparative assessment of value chains has previously been noted as a problem in which many competing permutations are usually present. For a complete analysis of the alternatives available to a FMCG company, all of these must be assessed. As discussed, for systems in which each spoke set has an equal number of constituents, the number of permutations is given by Figure 4-1. However, real life value chain assessments are unlikely to present such an idealised scenario. Equation 4-13 details the method through which the number of possible hub and spoke permutations is calculated for an assessment with a single hub and asymmetrical spoke distribution, in essence, this is the product of the spoke set sizes.

$$Value\ Chain\ Permutations\ Present\ (P) = \prod_{s=1}^{n} (j_s)$$

Equation 4-13 - Calculation of the number of possible value chain permutations in a given problem. Where, n is the number of spoke sets present within the assessment, and j_s is the number of spokes within set s.

This process delivers an inventory where each rows details a unique value chain permutation. The decimal spoke IDs (exemplified within Figure 4-10) should then be used to succinctly track the spokes active in each permutation. An example is shown in Table 4-11 for a two-indicator (a and b) problem with three spoke sets, each with two available constituents (Using Equation 4-13; $P = 2 \cdot 2 \cdot 2 = 8$)

Table 4-11 – Permutation definition for a problem containing three spoke sets, each with two constituents. The active spoke's objective indicator scores are given in the right-most six columns relative to their local functional unit.

Permutation ID	Hub Spoke Interface Options			Active Spoke Objective Impact Indicator Result					
	Spoke Set 1 ID	Spoke Set 2 ID	Spoke Set 3 ID	S1,Ia	S1,Ib	S2,Ia	S2,Ib	S3,Ia	S3,Ib
1	1.1	2.1	3.1	$I_{1.1,a}$	$I_{1.1,b}$	$I_{2.1,a}$	$I_{2.1,b}$	$I_{3.1,a}$	$I_{3.1,b}$
2	1.1	2.1	3.2	$I_{1.1,a}$	$I_{1.1,b}$	$I_{2.1,a}$	$I_{2.1,b}$	$I_{3.2,a}$	$I_{3.2,b}$
3	1.1	2.2	3.1	$I_{1.1,a}$	$I_{1.1,b}$	$I_{2.2,a}$	$I_{2.2,b}$	$I_{3.1,a}$	$I_{3.1,b}$
4	1.1	2.2	3.2	$I_{1.1,a}$	$I_{1.1,b}$	$I_{2.2,a}$	$I_{2.2,b}$	$I_{3.2,a}$	$I_{3.2,b}$
5	1.2	2.1	3.1	$I_{1.2,a}$	$I_{1.2,b}$	$I_{2.1,a}$	$I_{2.1,b}$	$I_{3.1,a}$	$I_{3.1,b}$
6	1.2	2.1	3.2	$I_{1.2,a}$	$I_{1.2,b}$	$I_{2.1,a}$	$I_{2.1,b}$	$I_{3.2,a}$	$I_{3.2,b}$
7	1.2	2.2	3.1	$I_{1.2,a}$	$I_{1.2,b}$	$I_{2.2,a}$	$I_{2.2,b}$	$I_{3.1,a}$	$I_{3.1,b}$
8	1.2	2.2	3.2	$I_{1.2,a}$	$I_{1.2,b}$	$I_{2.2,a}$	$I_{2.2,b}$	$I_{3.2,a}$	$I_{3.2,b}$

The objective indicator results for each of the hub spoke interfaces are appended to the right-hand side of the table. Derivation and data entry to this table is, in itself, a potentially time intensive procedure. However, if carried out in excel, this can be resolved through automation using ‘Power Query’ (Python, R, or other methods are also applicable). With this table compiled for all possible value chains, indicator aggregation can be approached to quantify the impact of each permutation.

For the LCA and TEA strands, the spoke’s objective impacts are multiplied by the interfaces reference flow, R_s (where s is the spoke set considered), specified within the hub’s data sheet. The results are subsequently summed using Equation 4-14 to generate the value chain permutation’s overall objective impact profile.

Equation 4-14 – Calculation of the overall LCA and TEA result for impact indicator j in each value chain permutation. Where, H_j is the hub’s indicator j result, n is the number of spoke sets present, I_{ij} is spoke set s’s active spoke i’s objective result for indicator j, and R_s is the reference flow at spoke set s’s hub interface.

$$Overall\ LCA\ or\ TEA\ Value\ Chain\ Indicator\ j\ Result = H_j + \sum_{s=1}^{n}(I_{ij} \times R_s)$$

Due to the risk-based approach to SIA impact characterisation, the strand requires a different aggregation procedure than that used for the LCA and TEA objective results. Scaling the social impact risk in terms of the hub spoke interface’s reference flow would deliver erroneous results, reflecting the fact that risk is not a function of flow magnitude. Consequently, in the social strand, indicator values are summed across the hub and spokes present, then divided by the number of assessment modules (n+1) to generate an unweighted average; this yields Equation 4-15.

Equation 4-15 - Calculation of the overall SIA result for impact indicator ψ in a given value chain permutation. Where, H_j is the hub’s indicator j result, n is the number of spoke sets present, and $I_{i,j}$ is spoke set s’s active spoke (i) objective result for indicator j.

$$Overall\ SIA\ Value\ Chain\ Indicator\ j\ Result = \frac{\left(H_j + \sum_{i=1}^{n}(I_{i,j})\right)}{n+1}$$

With the deployment of these aggregation procedures the overall objective impact of every value chain permutation is known for all indicators assessed. These results are directly comparable to traditional LCAs and TEAs, while simultaneously incorporating the third SIA strand. Aggregation of the value chain components in this fashion allows for the rapid and efficient generation of ‘global’ LCIA results, significantly reducing workloads in comparison to existing methodologies or frameworks. These objective results are, at this point, fully ringfenced. This is done to prevent interference from the subjective aspects of the assessment, heralding from the MCDM module. Without this step, the final results would lose objectivity and any potential for ISO compliance.

4.5.3.8 Overall Ranking & Selection of Value Chain Permutations

Having calculated and ringfenced the objective assessment results, the value choices and indicator weightings derived from the MCDM module can be incorporated in parallel to rank the compiled permutations. This allows for the prioritisation of the decision maker or FMCG companies values, without suppressing the true, or objective, results.

To begin this ranking process, the AHP-TOPSIS derived local spoke rankings (within their set) are examined. Revisiting the hypothetical assessment scenario in Section 4.5.3.7, Table 4-11, the objective indicator values in the right most columns are replaced with the locally calculated subjective sustainability score of each (calculated in Section 4.5.2.4 through Equation 4-7, Equation 4-8). The result of this approach is shown in Table 4-12.

Table 4-12 – Aggregation of active spoke scores for each value chain permutation. Where $S_{s,\zeta}$ is the local normalised spoke score of set s and spoke ID ζ.

Permutation ID (ε)	Hub Spoke Interface Options			Active Spoke Normalised Subjective Sustainability Score			Value Chain Overall Subjective Sustainability Score ($\bar{S}_{\varepsilon}$)
	Spoke Set 1 ID	Spoke Set 2 ID	Spoke Set 3 ID	Spoke Set 1	Spoke Set 2	Spoke Set 3	
1	1.1	2.1	3.1	$S_{1,1.1}$	$S_{2,2.1}$	$S_{3,3.1}$	$\bar{S}_1$
2	1.1	2.1	3.2	$S_{1,1.1}$	$S_{2,2.1}$	$S_{3,3.2}$	$\bar{S}_2$
3	1.1	2.2	3.1	$S_{1,1.1}$	$S_{2,2.2}$	$S_{3,3.1}$	$\bar{S}_3$
4	1.1	2.2	3.2	$S_{1,1.1}$	$S_{2,2.2}$	$S_{3,3.2}$	$\bar{S}_4$
5	1.2	2.1	3.1	$S_{1,1.2}$	$S_{2,2.1}$	$S_{3,3.1}$	$\bar{S}_5$
6	1.2	2.1	3.2	$S_{1,1.2}$	$S_{2,2.1}$	$S_{3,3.2}$	$\bar{S}_6$
7	1.2	2.2	3.1	$S_{1,1.2}$	$S_{2,2.2}$	$S_{3,3.1}$	$\bar{S}_7$
8	1.2	2.2	3.2	$S_{1,1.2}$	$S_{2,2.2}$	$S_{3,3.2}$	$\bar{S}_8$

Having compiled the local subjective sustainability scores of all spokes, ranking of the value chain permutations can begin. To this end, an average is taken of the local subjective sustainability performance scores (using Equation 4-16), exclusive of the hub, giving *n* contributing values. The hub is not included as it is not selected from alternatives within the framework and therefore has no normalised performance score. Spokes' contributions to this average are not weighted on the basis of each spoke set's reference flow (R_i). This methodological decision was taken to ensure that any assessments with a dominating spoke set (those with a reference flow of large relative magnitude) do not exhibit a saturation effect around the selection of that spoke. In such an event, the framework would rank all permutations with a good performance in that spoke highly, failing to meaningfully evaluate performance differentials present in the other sets.

Equation 4-16 – Calculation of the overall value chain permutation performance score ($\bar{S}_{\varepsilon}$). Where $\mathcal{E}$ is the evaluated permutation's ID, n is the number of spoke sets present in the assessment, and $S_{i,\zeta}$ is the local normalised spoke score of set i and specific spoke ID ζ.

$$Value\ Chain\ Overall\ Subjective\ Sustainability\ Score\ (\bar{S}_{\varepsilon}) = \frac{\sum_{i=1}^{n}(S_{i,\zeta})}{n}$$

After application of Equation 4-16 to the compiled value chain permutation inventory (Table 4-12), an overall subjective sustainability score ($\bar{S}_{\varepsilon}$) between zero and one is obtained for each competing alternative (Equation 4-16). This column ($\bar{S}_{\varepsilon}$) of Table 4-12 can be used to rank the permutations in accordance with their alignment to the decision maker's value choices prescribed through AHP-TOPSIS. While the highest scoring permutation may not infallibly deliver the best available objective indicator result present, it minimises the impacts across all indicators while focussing more intensely on areas deemed important by the FMCG company.

4.6 Discussion

What is clear from the work carried out herein is that the needs of a FMCG company incentivise a unique, sustainability assessment framework. As identified in the early stages of this chapter, the safeguarding of the principles laid out by the ISO 14040 standards are critical to continuing the delivery of robust and objective assessment results (in the LCA strand and beyond). This has been a driver during the development framework, primarily aiming to deliver meaningful, transparent, and actionable insights around the likely impacts of FMCG value-chains. However, beyond this, several application specific considerations, such as the requirements of sustainability assessments within a FMCG setting, are unpacked in search of further framework utility. The following discussion examines the progress made, and difficulties encountered, in terms of each of the objectives specified in Table 4-1. A critical analysis of the framework and its functionality is primarily approached in the discussion of the 'aggregation of methodological components within an assessment framework' (Section 4.6.4), preceding sections target the evaluation of the efficacy with which key principles and methodologies were identified and incorporated.

4.6.1 Alignment to ISO 14040's Guiding Principles

Revisiting the first objective, laid out in Table 4-1, the degree of alignment achieved with respect to the ISO standards guiding principles can be examined in detail. The result of this homologation effort is chronicled from ideation within the framework's guiding philosophy (Section 4.3). Seven guiding principles established by ISO are identified within the literature review (Section 3.4.1.1) and listed in the first column of Table 4-13. The second, right hand column, gives evidence of the framework's adherence to, and incorporation of, these principles.

Of these, the first principle is the adoption of a lifecycle perspective. This is clearly evidenced within the framework through its ability to assess a broad range of scopes depending on the choice of system boundaries and spoke sets to incorporate. However, perhaps the most demonstrable example is the ability to conduct a full cradle-to-grave impact assessment. Through such an application, not only is the environmental lifecycle fully defined, but also the economic and social counterparts; holistic assessments deliver an even broader lifecycle perspective through the quantification and identification of burden shifting. Table 4-14 details the ways spoke set inclusion can be tailored by practitioners to examine classical assessment scopes.

The second principle is an environmental focus. This is clearly achieved through the incorporation of a robust LCA methodology and reporting procedure. However, the integrated nature of the assessment develops upon this focus to include economic and social aspects. In the broader context it is believed that the holistic stance of the methodology will support the long-term improvement of processes' environmental performance, mitigating the risk of overcompensation and the resulting burden shifting, an issue that may eventually threaten to reverse environmental benefits in the pursuit of economic or social factors if not carefully managed. Furthermore, if a FMCG company is particularly interested in an environmental assessment, the framework permits independent strands assessments, while simultaneously delivering the same workload reductions realised through the developed MCDM and aggregation procedures.

Table 4-13 – List of the ISO 14040 guiding principles and evidence for their attainment within the developed framework.

ISO 14040 Guiding Principles	Evidence for the Framework's Attainment of ISO Guiding Principles
A life cycle perspective	- The framework achieves applicability to assessment scopes ranging from gate-to-gate to full cradle-to-grave. - Adherence to ISO's system boundary philosophy
Environmental focus	- Assessments independently evaluate each of the three strands via a harmonised methodology based on LCA relevant best practices. - Strand results can be viewed in isolation allowing for a solely environmental, economic, or social focus if desired.
Relative approach and functional unit	- Relativity is oriented around a defined product selected by the FMCG company (typically evaluated on a mass basis) - The functional unit approach of ISO 14040 and the GCI guidelines is applied to each spoke set and overall assessment individually, facilitating the modular inter-operability of each hub and spoke LCI. - Spokes are examined and selected relative to their local set, or cohort.
Iterative approach	- The process through which constituent hub and spoke LCIs are generated is directly adopted from the ISO 14040 standards, facilitating iteration and improvement of factors such as data quality, system boundary, etc. - Assessment expansion is simple and convenient, only requiring the addition of new/recycled spoke data sets.
Transparency	- The transparency achieved by the ISO standards methodology have been fully translated to the TEA and SIA strands, requiring the use of quantified and repeatable characterisation procedures. - All hubs and spokes used within the assessment are characterised fully within their respective standardised data sheets to avoid any ambiguity.
Comprehensiveness	- Generation of impact scores for an exhaustive range of value chain permutations. - The framework can be utilised for a wide range of assessment goals, including varied system boundaries, indicator selection, functional unit, etc.
Priority of scientific approach	- Utilisation of widely accepted and utilised LCA and TEA characterisation models to generate objective impact indicator results. - Adoption of quantifiable and repeatable social impact characterisation models that reduce the scope for the introduction of practitioner subjectivity and bias. - Implementation of a consistency scoring procedure within the MCDM module to verify the validity of decision maker value choices and the resulting indicator weighting.

Table 4-14 – Assessment components required to achieve different scopes.

Assessment Scope	Input Spoke Set Assessment	Hub Assessment	Output Spoke Set Assessment
Gate-to-Gate		✓	
Cradle-to-Gate	✓	✓	
Gate-to-Grave		✓	✓
Cradle-to-Grave	✓	✓	✓

Benefits realised through ISO's relative approach and functional unit are expanded upon within this framework. Definition of both global and local functional units allow for greater interoperability of datasets between assessments, permitting a 'plug and play' approach to system modelling similar to that seen in Ecoinvent's data structure. Such clear demarcation of constituent LCI boundaries presents opportunities for their seamless secondary utilisation in assessments of value chains requiring the same input material. Within the setting of FMCG value chains this is of significant value as each modular assessment can be shared or updated within the organisation, expediting subsequent assessments while contemporaneously ensuring attainment of 'oranges to oranges' comparative studies. The iterative approach around which LCA has been developed is also safeguarded. Deployment of the modular LCI/LCIA structure allows for refinement of aspects such as data quality and system boundaries at either the spoke, spoke set, or assessment level. This delivers a previously unseen degree of flexibility.

Transparency, the fifth of ISO's guiding principles, was a key focus during the framework's development phase. This is reflected through the integration of recognised methodological components such as the LCA and TEA characterisation methods, four phase format and the focus on open-source literature data. Beyond this, the use of standardised hub and spoke data sheets contribute significantly to the transparency achieved by assessments. Through these, the mass balances, energy requirements, temporal and spatial relevance, and system boundaries are clearly outlined. By transparently communicating these aspects of the assessment, stakeholders can clearly identify any incongruencies when comparing the generated results to those from a different assessment. Within LCAs seen in literature, the system boundary is often defined vaguely, leading to opacity and miscommunication about LCIs and technologies' potential benefits.

As a consequence of the aggregation procedure employed within the methodology, the hub and spoke framework is not only comprehensive, but demonstrably exhaustive. Quantified objective and subjective impact assessments are delivered for all possible value chain permutations, not just those identified as having significant potential for improved performance. This thorough examination of the meta-system results in greater insight generation, as well as higher certainty around the relative performance of a given value chain alternative. These insights facilitate more informed decision making at the R&D level, an important aspect of FMCG value chains, exhibiting rapid development and deployment cycles. By targeting holistic assessments, the framework significantly expands upon the comprehensiveness of the ISO standards by quantifiably examining inter-strand burden shifting; the first true example of this for FMCG and holistic applications.

The final ISO guiding principle is the adoption of a scientific approach. With integration of the social strand comes notable challenges in this respect. The complexity of social impact pathways has so far stifled the development of characterisation models equivalent to those seen in LCA and TEA; a fact revealed within the preceding literature review (Chapter 3). Where the environmental impacts (either mid or endpoint) of a given emission remain largely the same, irrespective of the location, social impacts are heavily dependent on geographical effects, manifesting themselves through the cultural, religious and socio-economic background of the groups present. This issue surfaces prominently within the frameworks impact characterisation procedure. LCA and TEA characterisation methods are adopted directly from literature and best practice within the field. To achieve the desired quantified holistic assessment, the derivation of a novel social impact characterisation method is required. In the absence of such work, the framework would remain incomplete and inoperable. This issue is tackled in Chapter 5, remedying the strand's methodological divergence to deliver what is believed to be the most scientifically robust holistic methodology seen to date.

4.6.2 Identification and Inclusion of Attributes Pertinent to FMCG Value Chain Oriented Assessments

Moving away from the ISO guiding principles, and back towards the objectives laid out at the beginning of this chapter, the identification of attributes required for the meaningful application of holistic sustainability assessment within the context of a fast-moving consumer goods company (Objective 2.2 within Figure 2-1) can be reviewed. Through the evaluation of literature, the key drivers, and requirements for success within FMCG value-chain are identified, informing, and expanding the frameworks development pathway. While several of these aspects, including the need to assess a large number of alternative value chains, were immediately apparent, factors such as the need for enhanced results communicability to consumers and decision makers were not. Furthermore, the 'obvious' requirements, once examined in full context, revealed much more nuance and inter-relation than initially expected. A prominent example of this is seen in the aforementioned consideration of the exceedingly vast number of potential alternatives (visualised through Figure 4-1). This, along with a detailed understanding of the 'problem structure', directly influenced the decision to adopt a hub and spoke network topology within the framework, delivering all desired methodological characteristics (Table 4-2).

This realisation and development opportunity is seized with both metaphorical hands, functioning as the axis around which the framework is compartmentalised. Initial examination of spoke sets as an independent local assessment allows for the addition or substitution of specific feedstock options without impacting neighbouring sets. The ringfencing of spoke LCIs also facilitates a 'plug and play' approach to interoperability, significantly reducing subsequent practitioner workloads.

Communication to non-practitioner decision makers and consumers is improved through the calculation of a single overall performance score in parallel to the objective indicators. This incorporates the value-choices of the FMCG based decision makers and is oriented around the relative objective impacts of competing LCI. The resulting approach simultaneously evaluates the objective impact profile and alignment to corporate strategy of each value chain permutation or alternative. While believed to be very valuable as a communication and decision-making tool, this overall score should be utilised with caution due to its inherent subjectivity. Where used, the value choice derived indicator weightings, and objective indicator results, must be presented in parallel to safeguard against potential greenwashing efforts and maintain transparency. Such greenwashing could easily be approached if decision makers assign high value to the technoeconomic indicators with little regard for environmental or societal factors; in such cases the overall value chain score may look close to optimal in spite of significant detrimental effects caused by mathematically incentivised burden shifting.

Further expanding upon this logic and concern, it is suggested that any consumer facing deployment of a value chain's overall performance score be based on an unweighted MCDM scenario (all indicators receive an equal weight). This prevents the introduction of performance biases originating from weightings based on corporate strategy. In scenarios where two competing assessments use different indicator weightings, comparability between the overall performance score's value is degraded significantly, favouring reliance on the more traditional objective results that are protected from subjectivity (discussed in Section 4.5.3.7).

Identification of a high TRL assessment focus reveals another aspect of the framework that demonstrates a FMCG orientation. In an industry dependent on reliable production rates and short lead times, low TRL processes are very rarely considered for adoption. Benefits are immediately realised when only considering TRL 8-9 processes, previously identified examples being the omission of performance optimisation predictions and the presence of more comprehensive and detailed literature data. However, these benefits come at the cost of a framework that is ill suited to the assessment of low to medium TRLs should that be desired. While not a unique issue within the broader field of sustainability assessment [111], it does constitute a methodological limitation. It is important to note that if a low TRL assessment was targeted, all other alternatives assessed should be of a comparable readiness level. Direct comparison of a high and low TRL process offers little in terms of insight owing to the significant uncertainty that accompanies data for pre-pilot technologies. Unexpected gains in efficiency, or overly optimistic projections, can significantly swing indicator performance in either direction as the development progresses through TRL's. When considering this work's setting and objectives, the focus on deployed technologies is a pragmatic and beneficial trait. It is proposed that in the event that low TRL processes gain traction within FMCG value chains, a second iteration of the hub and spoke framework considering the specific considerations of low TRL value chain development should be targeted.

4.6.3 Selection and Integration of an Appropriate Multi Criteria Decision Making Technique

Identification of the most appropriate and valorising methodology was approached systematically through a literature search and specification of selection criteria based on the requirements on a FMCG company laid out in Section 4.4. The early selection of MADM over MODM significantly reduced the number of options to assess and resulted in a more thorough analysis. Removal of MODM techniques from the selection process was deemed appropriate as they are designed to examine undefined or continuous alternatives, the polar opposite to the problem typology observed within FMCG sustainability assessment. Rather than optimising a continuous set of objective functions, the framework must identify the best option available from a set of discrete alternatives with well-defined performance parameters. The use of MODM appears better suited to the process optimisation phase of low TRL technologies within R&D, a context in which the properties of the product can often be altered on a dynamic basis by manipulating operating conditions.

MCDM, and MADM in particular, is a growth area within the broader field of sustainability assessment. As identified earlier, inclusion of decision-making support within sustainability assessments has grown from ~0.2% of publications to ~0.8% in fifteen years [203]. This small but proportionally significant increase captures the acknowledgement of the value addition that MCDM delivers within LCA, TEA, and SIA's multi-variate problem spaces. With often significant indicator counts it was deemed crucial that the framework include a robust and repeatable indicator weighting derivation and subsequent selection of the best performing alternative within the available pool. Simple evaluation of decision maker value choices, and weightings, via the WSM was deemed insufficient in this regard. Work by Halford, *et al*. identified an inability of humans to accurately weight and evaluate problems with more than four variables without assistance from more complex mathematical techniques [206].

To identify and select a fitting methodology, a systematic literature review was conducted. Due to the scope of this project, the evaluated methods could not be exhaustively applied in parallel, and the differences in recommendations examined. Consequently, a set of seven methodological attributes were identified (Table 4-3), the attainment of which would deliver a capable and context appropriate MCDM methodology. Identification of alternative techniques and their fulfilment, or lack thereof, of the specified attributes was approached through a systematic literature review outlined in Section 4.5.2. This process identified 72 publications and 13 techniques, from which a hybrid AHP-TOPSIS approach was precipitated.

The selected approach separates the MCDM process into two halves, the derivation of weightings, and the ranking of competing alternatives. This strategy eliminates the weaknesses of both AHP and TOPSIS while maintaining, or in some respects, augmenting their strengths. In the setting of a FMCG company, approachability to non-practitioners is vital. AHP delivers this through the use of an easy to interpret scoring scale (Table 4-8) and straightforward procedure. The hierarchical structure of AHP also helps to reduce the workloads imposed on the decision maker by considering assessment strand and constituent indicator weightings independently, reducing the number of pairwise comparisons required by up to 68.63% [203]. Through this format, the decision makers and practitioners have efficient control over the weighting procedure. This is exercised through the availability of several calculation approaches, allowing for rapid weighting calculation based on decision maker value choice, indicator density, or uniformity. Furthermore, the frameworks mathematical integrity is ensured by the presence of a consistency check across the decision maker's AHP inputs. Conflicting value choices will be identified and prevented from progressing through the following framework modules. The overall effect of this consistency check is the prevention of erroneously calculated weightings from reaching the TOPSIS module and delivering incorrect value chain recommendations based on conflicting value choices. Such misleading insights would, at best, result in inefficient value chain selection and misalignment with corporate strategy. However, in the worst-case scenario, it may deliver recommendations that culminate in the poor allocation of development efforts or result in detrimental real-world impacts relative to other competing alternatives.

The tiered AHP structure realises an additional benefit, the assessment of independent strands. If a decision maker was to apply 100% of the tier one (strand level) weighting to, for example, LCA, the holistic assessment is transformed into a more traditional single stranded assessment. Similarly, double stranded assessments are possible by assigning only one strand a zero weight. While this nullifies the holistic nature of the developed methodology and fails to fully utilise all of the data within the standardised datasheets, in specific applications such as generating LCA data to support eco-labelling claims or comparison of many permutations, benefits are realised. Ultimately, this capability delivers a more flexible assessment structure than those previously available. However, with this comes the requirement that practitioners remain vigilant of the MCDM calculation option and value choice inputs provided by any non-technical decision makers and evaluate any unintended impacts on the final recommendations via consultation and interpretation of the objective results.

Even with the tiered AHP structure, assessments with many indicators may experience difficulties around the consistency of decision maker value choices and the resulting consistency ratio. As outlined by Saaty [161] [207], as the number of criteria within a single AHP matrix rises, an acceptable consistency ratio is increasingly difficult to achieve. The specification of a 9-point scale, against which the decision maker evaluates the pairwise comparisons, offers utility in terms of a greater degree of preference differentiation; however, it also exacerbates the issue of scoring consistency. Consequently, in assessments examining a large number of indicators within any given strand may benefit from a reduced 5-point scale to simplify and expedite the AHP weighting procedure. Despite this slight methodological deviation from the proposed nominal framework application, the objective indicator results remain fit for comparison against assessments utilising the original 9-point scale; furthermore, the same hub and spoke data sheets can be utilised interchangeably.

With the decision makers AHP inputs completed and checked for consistency, the resulting weightings are fed into TOPSIS where the alternatives are subjectively ranked. At this point, no further decision maker input is required, delivering a framework that is as intuitive and streamlined as possible. TOPSIS forms an ideal 'back-end' for the MCDM section of the framework due to its ability to evaluate a large range of alternatives in n^{th}-dimensional problem spaces. Furthermore, the technique is seen relatively commonly (in a non-hybridised form) within sustainability assessments that employ MCDM (see Figure 4-5), increasing the likelihood that practitioners have experience or knowledge of the TOPSIS methodology.

4.6.4 Aggregation of Methodological Components Within an Assessment Framework

Within the guiding philosophy laid out in Section 4.3, the overall approach to the framework development focussed on the selection of appropriate constituent methodological decisions (LCI format, characterisation methods, MCDM technique, etc.). When evaluating the resulting architecture (Figure 4-9) the benefits realised by this are clear. The assessment workflow is logical, sequential, and easily partitioned. It is believed that this presents significant value addition to the targeted audience, FMCG companies. Many aspects of the framework, including but not limited to the AHP-TOPSIS MCDM module, can be standardised in template form and readily applied to new assessments. This, combined with the workload reduction realised through the use of ring-fenced and standardised spoke LCIs, and a tiered AHP structure, delivers a novel methodological tool in which complex value chains can be rapidly assessed on a comparative basis.

In contrast to these standardised aspects, the framework retains the practitioner-oriented flexibility delivered by the preceding methodologies. This ensures applicability to a broad range of goals, scopes, and product systems. Primary examples of practitioner led aspects include the selection of indicators, normalisation procedures for the objective indicator values within each spoke set, and the development of LCIs. Of course, this also prevents the opportunity for bias, be that conscious or unconscious. However, the nature of the assessment, being aligned with the ISO standards, means that the constituent LCI's can theoretically be peer reviewed, eliminating a large proportion of these concerns.

The main weakness identified within the framework is the elevated complexity of the LCI sensitivity analysis procedure. Where for a standard LCA and TEA key data inputs are identified and varied by +/-*x*% and +/-*y*%, the developed framework is not so straightforward. Due to the decentralised nature of the hub and spoke LCIs, the variables values must be changed independently for each. While this is more workload intensive, the general procedure is the same, but requiring of repeat application. As the number of spokes, or spoke sets, increases, this task grows linearly in magnitude. A solution, or at least partial solution, to this issue may be found through the selection of key variables with high likelihood of inclusion within an assessment's sensitivity analysis. Once identified, these input variables and their associated data points can be scaled by +/-*x*% and +/-*y*% and the resulting impact profiles tabulated within the spoke's data sheet for later use in sensitivity analyses. While this is not an insignificant methodological augmentation, the process can be automated within an excel based LCI file once the relevant variables are chosen. A primary consideration in the resolution of this weakness is the effectiveness of the assessment's standardised data sheets; addition of significant quantities of data risks jeopardising the efficiency of assessment conduction, as well as producing unwieldy data sheets.

Another area ripe for future development is the normalisation procedures utilised within the local spoke sets to prepare the ring-fenced objective indicators for utilisation within the AHP-TOPSIS module. As identified in Section 4.5.3.4 and Table 4-7, the magnitude and distribution of the constituent spokes' indicator results can negatively impact the efficacy of the suggested normalisation procedures (Equation 4-7 and Equation 4-8). Where practitioners are concerned about this phenomena, alternative normalisation procedures can and should be employed, a promising example being utility curves. However, the superseding approach must be documented for transparency in terms of inter-assessment comparative assertions and repeatability.

With a full framework architecture detailed, it is clear that one of the key strengths is the selection of a hub and spoke network topology in conjunction with the development and specification of a concise hub/spoke interface. This methodological development expands upon the idea of an intermediate flow, utilised commonly within LCA and TEA. Furthermore, it delivers a degree of interoperability previously unseen beyond the Ecoinvent database.

Examining Figure 4-9, it is seen that the indicator weighting procedure is an optional methodological pathway. This is facilitated by the objective indicator results early ring-fencing. Through this approach, in the absence of decision maker and AHP derived weightings, TOPSIS is not applied to rank the available permutations. Such assessments therefore deliver only the objective indicator results. While these are of significant value, and certainly of more use to the practitioner and broader academic community, the lack of ranking procedure results in challenging selection of a value chain from the available alternatives. This could be circumvented, or at least aided, by filtering the final results table to examine the best performing alternative relative to each assessed indicator. It is important to note that this approach will not quantitatively examine the trade-offs in indicator performance. An alternative strategy is therefore proposed in the absence of decision maker value choice inputs, using uniform weightings to prevent preferential handling of any given indicator. This approach would deliver an unweighted ranking of the value chain permutations' overall performance, mirroring the consumer facing version of the methodology discussed in Section 4.6.2.

The final point of discussion identified within the chapter is the current lack of impact pathway based social impact characterisation models. A fact that has historically significantly hampered the effective harmonisation of the three assessment strands, and enforced the continued developmental stagnation of SIA. Also noted within the literature review, this constitutes a significant gap in both current knowledge and capability. Owing to this absence from open literature, a sizable hole can therefore be found within in the framework's architecture. Consequently, instead of adopting a reference scale approach and compromising the target of fully quantified results, as is done by McCord, *et al.* within the triple helix framework [7], it was decided to develop an initial set of impact pathway characterisation models (tackled in Chapter 5). This represents a significant challenge in terms of the availability and quantity of data required. However, this effort should be rewarded with a more repeatable, transparent and data driven approach than any preceding alternative.

4.7 Conclusion

Within this chapter of work a novel framework for the holistic sustainability assessment of FMCG value chains was theorised and developed. Through the adoption of the ISO 10404 standards as a foundation, and drawing heavily on the previous advances of the triple helix framework, a robust and broadly applicable methodology is realised. In addition to this, attributes of value in the FMCG context are examined through literature, revealing the need for an approach that can handle very large numbers of alternatives, and that can deliver recommendations aligned with the organisation's broader corporate strategy. The framework's other valorising characteristics with respect to FMCG applications will not be reiterated owing to their inclusion within Sections 4.4 and 4.6.

The delivery of these two key attributes was achieved through the adoption of hub and spoke network topology, efficiently handling the presence and later addition of assessment alternative, followed by the selection of a highly appropriate and reliable MCDM technique. As seen commonly with computer engineering, the network topology provided the backbone and structure of the developed framework. Furthermore, it is proposed, based on the systematic examination of competing options, that the hub and spoke structure is the only viable option for the targeted use case. This has allowed for a highly compartmentalised methodology, acting on key aspects of the assessment in isolation before handing off relevant data to other modules. The constituent modules within the framework can be summarised through the following list;

- Impact characterisation approach
- Inter-module umbilical specification and data sheet development
- Lifecycle inventory generation and analysis
- Spokes et normalisation and performance matrix generation
- Decision maker's indicator weighting calculation
- Ranking and selection of value chain permutations
- Aggregation of hub and spoke modules

While this seems like an extensive and lengthy list, each component is crucial to delivering robust assessments that adhere to the current best practices and reflect the needs of FMCG companies. Furthermore, as highlighted in the discussion, this approach allows for the highly effective division of labour. Practitioners can work on each component in series or parallel, subsequently aggregating them together to deliver a functioning assessment.

Beyond structural novelty, the framework is the first holistic sustainability assessment methodology to mandate exclusively quantified impact pathway based characterisation models. Adoption of this approach within the social strand significantly bolsters the reproducibility of any given assessment. By ensuring that any practitioner, given the same LCI data, arrives at the same numerical value for the risk of negative impacts, a persistent methodological shortcoming is addressed.

Within this chapter it has also been demonstrated, through Figure 4-11 and Section 4.5.3.2, that aspects of the methodology can be standardised for use in a template form. Within the framework, the conduction of AHP is tackled in an approachable way, catering to a non-practitioner audience. Through the adoption of MS Excel as a canvas, recognising the intended use of the framework as a tool within FMCG companies, a demonstrator set of AHP matrices were presented (Figure 4-11). In this, the assignation of calculation methods, and pairwise comparison scores, is approached via drop down menus presenting the available options to the user. The evaluation, acceptance, or rejection of decision maker inputs based on value choice consistency is also deemed a beneficial for both results quality and ease of use. The approachability of the user facing modules, and their 'packaging', directly heralds from the identification of corporate decision makers as a key user and stakeholder. Through this, a novel and powerful tool for the evaluation of FMCG value chains and their associated impacts is realised.

Ringfencing of the objective impact results represents another strength of the framework, utilising the subjective results for the selection of value chain components without losing sight of robust impact characterisation. Delivery of these aspects in parallel sets this framework apart from other alternatives such as the ILCD handbook and GCI's Integrated LCA and TEA guidelines [21] [39]. This is perhaps the greatest direct value addition to FMCG companies, extending vicariously to their external stakeholders. By allowing organisations to tailor their sustainable development to the needs of their business model and strategy, there is more incentive for action. This initially appears to be easily exploitable, facilitating the targeting of areas seen by leadership as 'low hanging fruit', prioritising cost-effective gains. However, as benefits are realised in these areas of the sustainability profile, any neglected aspects or indicators become more apparent, self-incentivising their own examination and improvement through a passive feedback loop. Robust reporting against a broad range of impact indicators, and this feedback mechanism, leave little room for stagnation in terms of progression towards sustainable industrial ecosystems. What remains to be seen is a proof-of-concept study (Chapter 6), applying the developed framework to an appropriate industrial use case, examining its performance and capability for insight generation.

5 Quantification and Characterisation of Social Impact Risk

The work within this chapter (excluding Section 5.2) has been published within Frontiers in Energy Research:

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Alex Newman -	Conceptualization, methodology, formal analysis, investigation, literature and data curation, writing, review and editing.
Rachael Rothman -	Supervision and review
Peter Styring -	Supervision and review.

5.1 Introduction

First attempted in 1996 by O'Brien, *et al*., social impact assessment (SIA) aims to systematically and repeatably evaluate the social effects of activities, policies, or legislation [29]. Alternatively, it can be defined as; "the process of identifying the future consequences of current or proposed actions, which are related to individuals, organisations and social macro-systems" [7] [95] [200].This is typically achieved by considering a diverse stakeholder portfolio containing relevant impact categories and indicators. The idealised outcome of a well-conducted SIA is the safeguarding, monitoring, and (in many cases) mitigation of social pressures associated with sustainable development. Many assessment frameworks for social performance have been proposed, the most notable being the United Nations' Sustainability Development Goals (UN SDGs) [208]. However, owing to the complexity of societal structures and human behaviour, accurate characterisation remains a field-wide challenge. Consequently, methodologies often incorporate practitioner judgement, or other sources of subjectivity, delivering qualitative or pseudo-quantitative results. In addition, most work focuses on the assessment of deployed activities, neglecting the pre-emptive assessment of proposed projects.

In a broader sense, SIA can be seen to represent one of three 'strands' within a holistic view of sustainability. Environmental, economic, and social factors must all be managed responsibly to deliver long-term sustainable practices. While environmental lifecycle assessments (LCA) and techno-economic assessments (TEA) are mature and standardised, social impact assessment (SIA) is still a relatively underdeveloped field. Attempts have been made to integrate the three strands, making significant headway in the form of the Global CO_2 Initiative's (GCI) combined LCA and TEA guidelines [39], and McCord *et al*.'s Triple Helix Framework [7]. Despite this progress, the lack of consistent, quantitative methodologies for SIA hinders the meaningful integration of otherwise parallel assessment strands. SIA's most notable shortcoming is a failure to provide transparent and repeatable characterisation models (CMs) to underpin impact indicator reporting. This issue has long been solved for LCA (and TEA), offering numerous robust and broadly accepted CMs such as CML2002, ReCiPe, TRACI, etc., each with specific use cases. SIA's lack of such quantitative impact characterisation prevents comparison between studies of competing technologies. Such an approach would also deliver increased transparency and reliability, aspects that are often dismissed within practitioner judgement-based scoring scales.

Procedural and methodological divergence within SIA, based on assessment focus (i.e., technology type or field), is necessary to accurately refine SIA practices; an observation mirrored in LCA via the ISO derived, and sector-specific, ILCD Handbook [21]. For instance, the assessment of deployed activities can be defined and supported by primary data, resulting in more straightforward impact pathway characterisation. In contrast, assessments of proposed future value chains, or low TRL technologies, cannot rely on such data and instead requires a risk-based approach that utilises only open-source data. In theory, this would identify red flags, allowing for the subsequent implementation of mitigation or monitoring procedures. SIA's current focus on deployed activities inherently contrasts its aim of supporting sustainable development, only quantifying impacts after capital investment and roll-out. However, if the activity or process is not intrinsically socially sustainable, deployment should be deferred until the root issues are resolved. Social sustainability should be attained, or projected, in the design phase, not retrospectively [203]. This philosophy requires a novel approach that does not rely on the primary data of a deployed technology or value chain.

Having identified this major gap in assessment capabilities, this paper focusses on the development of SIA impact characterisation in the context of carbon dioxide utilisation (CDU). With increasing cultural and societal relevance, and offering a partial answer to the climate crisis, CDU is a field in urgent need of such pre-deployment SIAs. Pieri, *et al*. conducted a review of CDU focussed sustainability assessments, concluding that none considered social impacts [102]. Following this, Chauvy, *et al*. approach meaningful consideration of SIA through examination of health and safety within CDU [209]. However, the consideration of social impacts in the field remains lacking. Early assessment would facilitate the minimisation or avoidance of negative social impacts prior to occurrence. After all, how efficacious can an environmentally sustainable technology be if it simultaneously generates negative social impacts?

The broad catalogue of CDU technologies seen in current literature, ranging from concrete manufacturing [210] to synthetic fuel production [211], harbour a diverse range of technology readiness levels (TRLs) and process types. This diversity demonstrates CDU's character as a rapidly developing and forward-looking field. However, it also makes the derivation and application of social impact characterisation methods a complex challenge. Even in cases where primary data is available, a rare scenario for low TRL CDU processes, it cannot be effectively used in comparative studies. Higher TRL processes will have benefited disproportionately from optimisation and scale-up efficiency gains when compared to theorised or bench scale alternatives at early R&D phases. Consequently, the development of flexibly applicable, non-TRL specific, CMs offers significant value to both CDU researchers and SIA practitioners. Furthermore, this high-level approach supports application to the full suite of CDU related technologies, circumnavigating the nuances related to specific technologies.

In addition, many CDU projects, particularly those at pre-deployment or low TRL phases, typically suffer from a lack of geographic specificity regarding operating location [39]. Often, only a vague targeted deployment region can be defined, informed by investment conditions, market forces, and labour requirements. However, macro level studies at continental or sub-continental resolution offer only vague insights. Consequently, the potential for negative societal impacts must be evaluated on a geographically meso-level, incentivising the development of methods adopting a national level scope.

The outlined issues demonstrate that CDU has sector specific needs that are currently neglected by broader, more general, social impact characterisation approaches. These can be succinctly summarised within six methodological requirements, or objectives;

1. Applicability to a broad range of technology types.
2. Pre-emptive identification of likely negative impacts associated with projects
3. A levelized and comparative consideration of diverse TRL ranges
4. Reliance on open source (non-primary) data
5. National (meso) level reporting resolution
6. Transparency and repeatability

The proposed national level red-flag philosophy, while less granular than approaches based on primary data, adds significant value at project inception or upgrade lifecycle phases. For instance, many CDU processes are highly energy intensive, a consequence of CO_2's inherent thermodynamic stability [212]. A SIA CM focussing on communities' access to electricity would augment an organisation's ability to determine whether existing energy infrastructure can be utilised, or, if on-site generation is required to safeguard local communities' energy needs. A plant requiring large amounts of grid electricity may not be socially sustainable if deployed in a country with a scarce or intermittent energy supply. However, if the project scope was expanded to include combined heat and power (CHP), photovoltaics, etc., sustainability may be realised. Through this approach, SIA does not exclude countries from consideration, but instead guides the targeting of remedial action. Furthermore, incorporating this philosophy within holistic assessments would allow detailed identification of burden shifting. In the previous example case, the abatement of social issues around electricity access would likely be reflected in elevated capital costs associated with CHP.

While not granting the same level of granular insight as LCA CMs, adherence to these six objectives delivers a value addition to organisations during the transition towards sustainable industrial ecosystems. Early identification of potential negative social impacts leaves time to remedy the causal factors, improving both long- and short-term sustainability profiles while removing the compromises associated with post-deployment optimisation. If conveyed effectively to key stakeholders, the results of such a red-flag assessment would support strategic industrial decision-making around CDU process deployment.

5.2 Aims and Objectives

Table 5-1 – Objectives for Chapter 5.

Objective	Specification
3.1	Evaluation of the current state of, need for, and feasibility of, quantified impact characterisation methods within social impact assessments.
3.2	Identify suitable open-source data sets to form the backbone of a reproducible and transparent assessments inventory.
3.3	Develop an initial set of quantified social impact characterisation models in which a range of data availability scenarios are covered.
3.4	Apply the developed characterisation models to generate example national level results and evaluate their effectiveness.
3.5	Determine and discuss the use cases in which such an assessment technique adds value to practitioners and decision makers.

5.3 Review of Literature

Previous reviews spanning a broad period reveal that SIA, constitutes the least standardised strand within sustainability assessment [30] [31] [32]. Impacts are most commonly reported relative to the UN SDGs (Sustainable Development Goals) [36] or GRI (Global Reporting Initiative) [35]. Assessments are typically carried out around deployed operations, generally neglecting processes residing in low TRL or R&D lifecycle phases [7], an issue realised to a lesser but still present extent in LCA. Beyond the UN and GRI approaches, Kühnen and Hahn [105] identify the UNEP (United Nations Environment Programme) and SETAC (Society of Environmental Toxicology and Chemistry) S-LCA guidelines, SAI (Social Accountability International) SA 8000, and ISO 26000 as alternate methodological options. However, the focus on deployed activities remains a common limitation [45].

A small number of sector-specific SIA approaches have been identified in previous literature [200], primarily focusing on the mineral [103] and mining [104] industries. Despite this specialisation, characterisation models analogous to those observed in LCA remain elusive. Furthermore, in the case of CDU-oriented SIA, there is no practitioner guidance around the quantitative handling of impact reporting. McCord, *et al.*, instead, propose practitioner-led reference scale approaches when aligning CDU-based LCAs, TEAs and SIAs [7]. While superficially aligning the three strands, the SIA 'scoring' methods introduce a much greater degree of subjectivity than their LCA and TEA counterparts. These shortcomings are due to both a lack of available data and an imperfect understanding of the macro societal systems through which impacts propagate. Where environmental impact pathways transcend national and cultural borders, social impact pathways are often dynamic, complex, and opaque. At this point, the field appears to have reached an impasse with respect to assessment specificity. Stakeholders desire more accurate and granular SIA results, with practitioners contemporaneously lacking the methodologies through which these must be generated.

UNEP and SETAC clearly define two typologies of impact characterisation: the reference scale (formerly called Type I or RS S-LCA) and impact pathway approaches (formerly Type II or IP S-LCA). Each have their merits and limitations, reflecting fundamentally different schools of thought and delivering a significant methodological bifurcation. Reference scale approaches aim to "assess social performance or risk", whereas the impact pathway approach assesses "consequential social impacts through characterising the cause-and-effect chain" [106]. Reference scales usually utilise a five-point scale against which practitioners score the performance of evaluated alternatives. However, these scales incorporate several sources of fuzziness and subjectivity. Examples include the assignment of criteria for each scoring level, the use of linear versus non-linear scales, and the qualitative nature of performance ranking against (usually un-quantified) statements. Furthermore, the approach generates very coarse results due to the five-point non-continuous scale. In contrast, the impact pathway approach is more analogous to methods seen in LCA, allowing for more seamless integration of the strands within holistic assessments. However, the previously noted complexities associated with impact pathway modelling result in broader adoption of the reference scale approach, a conclusion mirrored in all major practitioner guidelines, including the latest CDU-focused framework, the triple helix framework [7].

Reference scale-based tools, such as the Social Hotspot Database (SHDB) [213], have been developed to aid practitioners in the conduction of SIAs. Indeed, the SHDB facilitates national level assessments scopes such as those targeted in this work. However, while valuable in many applications, the adoption of reference scale approaches to impact characterisation falls short of the methodological counterparts seen in LCA and TEA; inherently facilitating the introduction of practitioner subjectivity or bias. If the complete and meaningful harmonisation of environmental, economic, and social assessment strands is to be realised, an impact pathway-based approach must be presented for use by practitioner, transcending the SHDB's offering.

Compounding this divergence in characterisation approach, the SHDB is pay wall protected. This puts it in direct conflict with LCA and TEA characterisation methods, provided free of charge in all examined cases (CML2002, ReCiPe, TRACI, etc). If SIA is to be adopted on an equivalent basis, freely accessible impact pathway characterisation methods must be available to practitioners who lack the backing of well-funded organisations.

Failure to provide this may result in SIA's stagnation within a second strata of assessments, requiring database licences that exclude small businesses and independent practitioners.

GreenDelta's PSILCA database [214] represents what is deemed to be the closest analogue to the CMs targeted within this work. However, despite being based on the UNEP and SETAC guidelines, and examining a comprehensive 15,000 sectors (excluding CDU) across a mixture of 69 qualitative and quantitative risk-based indicators, it is designed to assess deployed processes and value chains. Therefore, the most pertinent gap in capability with respect to CDU related SIA, pre-deployment assessments, remains un-tackled. Furthermore, the indicator results are reported against a discrete qualitative scale (based on quantitative background calculations). This consequently fails to communicate social impact risks on a continuous basis, instead utilising reference-scale-like scoring points (low risk, medium risk, high risk, etc.). In addition to these factors, and similarly to the SHDB, PSILCA is also a paid product, resulting in the same accessibility issues as previously noted. Finally, the examination on a sector specific basis adds little value to CDU projects as it is not currently recognised as an independent industrial sector within PSILCAs methodology [214]. Owing to their surface level similarities, the PSILCA CMs will be compared to those developed in this paper within the discussion.

A secondary methodological divergence within SIA thinking can be observed in the handling and characterisation of positive social impacts. UNEP and SETAC propose their classification under three categories [106]: positive social performance going beyond business as usual [215], positive social impact through presence [216], and positive social impact through product utility [217]. These classifications again focus on deployed technologies, requiring detailed knowledge of the local communities. A majority of SIA methodologies, however, focus only on negative impacts [106]. While the argument can be made for the need to include positive impacts, the decision should be handled on a case-specific basis; their inclusion should enhance the insights delivered by a given assessment, not dilute the resolution at which potential negative impacts are examined.

The literature review's findings show that no CDU or value chain-oriented SIA guidelines further the development of impact pathway approaches. This paper therefore proposes that more emphasis should be placed on the impact pathway approach, aligning its development phase with reference scales to deliver more quantitative results. Additionally, impact characterisation through mathematical methods offers a remedy to currently observed subjectivity and repeatability issues.

5.4 Methodology

As identified through the literature review, impact pathway-based SIA lags behind its reference scale counterpart, both in terms of research effort and maturity. Consequently, herein we target the generation of initial open-source impact pathway CMs. The approaches developed primarily focus on applications concerning comparative assessments of CDU value chains, tackling the specific challenges identified through the literature review and building upon McCord, *et al.*'s triple helix framework. However, where McCord, *et al.* deploy a "qualitative scoring methodology based on quantitative and semi-quantitative data" [7], this approach targets purely quantitative assessment. The methodology aims to highlight elevated social impact risks based on deployment country. Generated results subsequently support the efficient allocation of resources for the pre-deployment prevention and mitigation of impacts through elevated due diligence and monitoring by the operating organisation.

Assessment indicators, clustered within stakeholder categories, are typically selected by the SIA practitioner from a broad pool, with 36 identified by Rafiaani, *et al*. [111]; this process draws on the assessment's goal and scope. Despite omitting impact pathway approaches, the triple helix framework offers significant advances in CDU SIA methodology in this respect. McCord, *et al*., building upon Rafiaani, *et al*.'s adaptation of UNEP and SETAC's guidelines to CDU technologies [111], streamline the stakeholder categories considered within assessments. UNEP and SETAC originally recommend a base set of five stakeholder categories [106];

1. Workers/employees
2. Local community
3. Society
4. Consumers
5. Value chain actors

These categories are subdivided into impact categories, subcategories, and associated impact indicators. The triple helix framework subsequently reduces this set to the consideration of only workers, local communities, and consumers [7], citing the irrelevance of other categories to CDU projects.

Owing to the scope of this work, the reduced set of stakeholder categories defined within the triple helix framework is adopted as a basis [7]. However, the consumer category can also be discarded when targeting comparative studies, providing an assessment scope aligned with cradle-to-gate LCA's; any products manufactured by competing CDU value chains should be identical, resulting in identical social impacts for consumers and no additional insights. This leaves consideration of only the worker (W) and local community (LC) stakeholder categories. Within these, seven indicators are selected for this proof-of-concept exercise. These reflect both a broad range of social issues, and typical difficulties experienced in the field (primarily data availability and reporting quality).

- Risk of Forced Labour (W)
- Risk of Child Labour (W)
- Occupational Health and Safety (W)
- Risk of Change in Access to Electricity (LC)
- Risk of Change in Access to Water (LC)
- Risk of Land Use Change (LC)
- Utilisation of Hazardous Materials (LC)

Due to the targeting of pre-deployment CM applicability, some common indicators such a fair wages or job creation cannot be evaluated. Without the specification of an operating location, their evaluation would result in problematic degrees of uncertainty or misrepresentation. To provide a pertinent example, as defined by UNEP and SEATC the job creation indicator sits within the local community stakeholder group [106]. This immediately represents a data resolution problem within national level assessments. Clearly, the societal impact of local job creation depends on the existing employment levels, skill availability, and economic activity within the specific local community that is to be impacted, immediately nullifying any insights gained from national level data. It should be recognised that a variation of this argument can be made for any national level impact indicator characterisation model. However, the seven indicators selected for the study, such as access to electricity (where installed generation capacity and national distribution grids introduce physical constraints), are primarily systemic in nature with less dominant regional drivers. Furthermore, job creation potential can vary significantly between population centres and rural areas, making a country-level assessment too broad to accurately predict employment outcomes. This is further compounded when considering the nature of jobs created. For highly skilled industries such as nuclear, it is not guaranteed that construction of a plant will provide the local community with jobs if they do not possess the requisite skills, instead favouring applicants from further afield. Factors such as these hinder several UNEP and SETAC's impact indicators in studies executed at the national level, negating any benefit of their inclusion. This resolution limited impact characterisation capability represents the first constraint of the proposed methodology. However, this is necessary in scenarios where the exact deployment region is unknown.

To facilitate an impact pathway-based methodology, stimulating and de-stimulating factors are identified for each indicator and systematically aggregated, delivering overall risk scores that highlight potential impact hotspots. The result is an approach closely aligned with the more thoroughly developed LCA CMs. Additionally, dependence on detailed process-specific data is avoided, aiding with technology comparisons over the diverse TRL range observed within CDU.

In the interest of transparency and reproducibility, only open-source data is utilised in the developed CMs. However, SIA-focused databases lag significantly behind their LCA counterparts, such as Ecoinvent [200]. Several characteristics were targeted within the data source selection: coverage, currency, reliability, and consistency. After consideration of multiple options, including ad-hoc collection, the World Bank is selected as the primary data source for CM development (also heavily utilised within PSILCA's methodology). With 189 participating countries and 12,000 social development projects [218], coverage is broad and reliable. Furthermore, constituent national-level data sets are updated regularly, with a majority reported annually. Reliability is safeguarded through the use of transparently audited data from partner organisations and governments. Finally, consistency is achieved inherently through the convergence of these prior factors. In some cases, secondary sources must be used to supplement the World Bank data; however, as discussed later, these often originate from partner organisations or constituent data sets. Once national level data for the stimulating and de-stimulating factors is collated, normalisation procedures are applied, delivering scores between zero and one through which the assessed CDU value chain alternatives' risk levels can be directly compared. This is a significant departure from the PSILCA methodology which utilises conversion to reference scales (discrete) in favour of normalisation (continuous).

Adhering to the red-flag approach, necessitated by the complexity of impact pathways, only negative social impacts will be considered. As previously identified, the evaluation and inclusion of positive impacts is a divisive issue within SIA. The developed CMs aim to highlight supply chain components with an elevated risk of negative social impacts, stimulating greater due diligence and monitoring efforts from the responsible organisation. Furthermore, positive social impacts should not be compensatory, as often seen in LCA and TEA. That is, positive impacts on one indicator or stakeholder group cannot be allowed to offset negative performance in another. From a moral stance, no stakeholder should wield the power to benefit one community at the detriment of another. Avoiding positive impact reporting removes such complications while simultaneously achieving the specified objectives.

Scoring directionality within SIA is also acknowledged by McCord, *et al*. as an important methodological decision [7]. That is, should negative social impacts be reflected through a high or low score? Directionality should be uniform across all indicators within an assessment, allowing for easily interpreted parallel reporting. In this methodology, countries with a high risk of negative social impacts are indicated by low scores, perceivedly the most intuitive approach.

Note to readers: ESI containing all utilised data and intermediate handing steps is available at Frontiers for simultaneous reference and the support of replication studies.

5.5 Method Development

In this section, the developed SIA CMs are laid out. The respective stimulating and de-stimulating factors, normalisation procedures, and attained geographic coverage are detailed. In the interest of conciseness, the complete datasets generated through these methods are not fully detailed in this paper, instead focussing on the G20 nations; however, the full results and utilised data sets for the 239 examined countries are provided within the supplementary material (MS Excel file found with the published manuscript at Frontiers in Energy Research).

5.5.1 Risk of Forced Labour

The risk of forced labour can be summarised as “work that is performed involuntarily and under the menace of any penalty. It refers to situations in which persons are coerced to work through the use of violence or intimidation, or by more subtle means such as manipulated debt, retention of identity papers or threats of denunciation to immigration authorities” [219].

The proposed CM evaluates the stimulating factors of current prevalence (per 1,000 population), and future vulnerability. This delivers keener insights than the sole consideration of prevalence, incorporating future exposure risk through the evaluation of additional aggravating factors. This national prevalence and vulnerability data is collected from a Walk Free Foundation report (WFF) [220], a partner and contributor to the World Bank database. Additional contributions were made by the International Labour Organization (ILO) and the International Organisation for Migration (IOM).

The estimated prevalence is evaluated using data collected by WFF through the Gallup World Poll. Complete reporting is observed for 167 of the World Bank’s 189 participating nations, providing a high degree of completeness. Estimated values range from 104.6 people in forced labour per 1,000 population (N. Korea) to people in forced labour per 1,000 population (Japan), full datasets are available in the ESI [220].

The prevalence values for each country (collected from the WFF report) are normalised within the set on a max-zero basis. This approach is selected to avoid assigning a score of 1 (indicating perfect performance) to a country with an estimated prevalence greater than zero. While this could conceivably cause the artificial grouping of countries' scores at the lower end of the scale, it is deemed essential to anchor the perfect score at zero prevalence. This decision only changes the highest normalised prevalence of forced labour (NPFL) score (for Japan) by 0.288% (from 1 to 0.997). The lower end of the scale moves dynamically with the highest (i.e. worst) national prevalence value. As a result, a global reduction in forced labour prevalence makes attainment of a positive score more challenging, incentivising continued improvement.

Equation 5-1 – Calculation of normalised prevalence of forced labour (NPFL). Where, PFL_{Max} indicates the highest national prevalence, and PFL_i indicates prevalence in country i.

$$1 - \frac{PFL_i}{PFL_{Max}} = NPFL_i$$

Equation 5-1 converts the full range of theoretical prevalence values to scores between 0 and 1 while correcting for desired directionality. The resulting upper and lower bounds for this normalised prevalence of forced labour (NPFL) are 0 and 0.99727 for N. Korea and Japan, respectively.

The second stimulating factor within the CM considers vulnerability to forced labour. This is a complex metric to quantify as unlike prevalence it cannot be directly measured. Consequently, the WFF's method evaluates several constituent risk stimulators, utilising procedures verified through an audit by Ernst and Young [220]. The full methodology behind WFF's quantification of vulnerability can be found in the referenced report [220]. In summary, an initial group of 35 risk stimulators were checked for collinearity, removing those with a significant correlation, defined as those with variance inflation factors (VIF) greater than 10 and tolerance below 1. 12 factors are removed in this process, eliminating the compounding effects and reduced sensitivity observed through the inclusion of multiple co-linear factors. The remaining 23 stimulators are grouped into clustered 'factors' through principal component analysis (PCA). The result is five overarching factors (listed below) that more approachably characterise a population's vulnerability to forced labour. An expert working group, selected by the WFF, was then consulted to assign weights to the five factors. This utilises the eigenvalues as weightings, indicating the amount of variance explained by each factor [220]. Those possessing greater eigenvalues, and therefore variance, explain a more significant proportion of the overall model and, thus, command greater weights. This process delivers the following factors and weights (detailed in brackets):

1. Governance Issues (5.76)
2. Lack of Basic Needs (3.422)
3. Inequality (2.233)
4. Disenfranchised Groups (2.092)
5. Effects of Conflict (1.938)

With the five constituent factors fully defined, weighted, and evaluated for each of the 167 countries considered, the raw national vulnerability scores can be calculated. This yields country-specific eigenvalue weighted values (EWV_i) through Equation 5-2.

Equation 5-2 – Calculation of the eigenvalue weighted value for country i. Where, F_{x_i} indicates the average value of factor x for country i.

$$\frac{(F_{1_i} \times 5.76) + (F_{2_i} \times 3.422) + (F_{3_i} \times 2.233) + (F_{4_i} \times 2.092) + (F_{5_i} \times 1.938)}{0.01 \times 5 \times 5.76 \times 3.422 \times 2.233 \times 2.092 \times 1.938} = EWV_i$$

This EWV represents a relative vulnerability score for each country, incorporating the 23 identified stimulating factors. However, this must be normalised, using Equation 5-3, to facilitate further use in conjunction with the national prevalence scores. This is defined as the Normalised Vulnerability to Forced Labour ($NVFL_i$)

Equation 5-3 – Calculation of the normalised vulnerability to forced labour for country i. Where EWV_{Min} and EWV_{Max} are the lowest and highest observed EVW across the assessed countries.

$$\frac{100 - \left(1 - \frac{99(EWV_i - EWV_{Min})}{EWV_{Max} - EWV_{Min}}\right)}{100} = NVFL_i$$

Having now defined and calculated the normalised national scores for prevalence and vulnerability, the overall indicator scores can be obtained through a simple average of the two values (Equation 5-4). This approach was adopted to assign equal importance of current prevalence and vulnerability; although, with time this weighting strategy can be revisited if supported by the results obtained through application cases. The national scores generated by Equation 5-4 provide a relative ranking of all considered countries between values of zero and one. Result of this calculation for the G20 countries gives the national risk profile detailed in Figure 5-3.

Equation 5-4 – Calculation of final risk of forced labour indicator score for country i.

$$0.5(NPFL_i + NVFL_i) = Risk\ of\ Forced\ Labour$$

5.5.2 Risk of Child Labour

As with the previous forced labour CM, prevalence and vulnerability are identified as stimulating factors. In order to clearly and consistently evaluate the prevalence of child labour, the classification requirements laid out by the United Nations Children's Fund (UNICEF) and the ILO are adopted (shown by Figure 5-1). This considers varied factors such as industry sectors, hazard, age, and duration, providing a widely accepted framework.

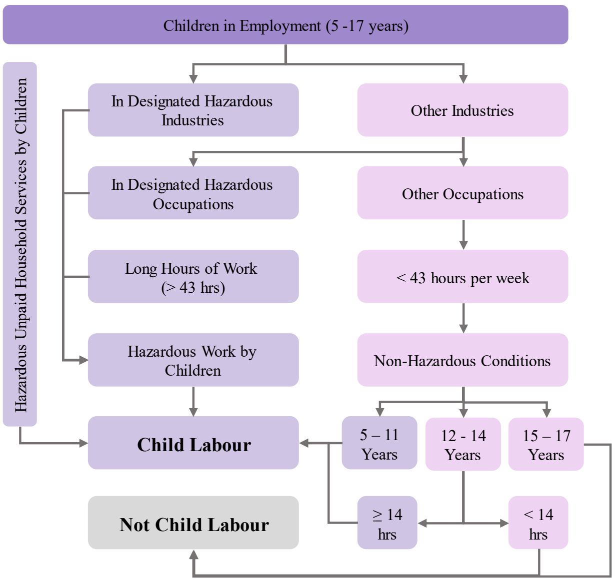


Figure 5-1 – Flow diagram showing the classification of what constitutes child labour. Adapted from UNICEF and ILO [221].

With a clear definition achieved, the quantification of national child labour prevalence is approached. However, data availability proves a challenge due to lacking geographic resolution. Rather than at the national level, data is presented in terms of the UN SDG regions listed below. This clearly reduces the granularity attained. However, the incorporation of vulnerability as a second stimulating factor augments the indicator's overall geographic resolution.

- Sub-Saharan Africa
- Central and Southern Asia
- Eastern and South-Eastern Asia
- Northern Africa and Western Asia
- Latin America and the Caribbean
- Europe and North America

Examining the reported prevalence data, all identified child labour between the ages of 5-17 is included. UNICEF independently report the prevalence of both hazardous and non-hazardous child labour as a percentage of the nation's population. For SIA CM development, both of these types are of significance. Additionally, the reported values are mutually exclusive, permitting their additive aggregation through Equation 5-5 without the risk of double counting.

Equation 5-5 – Aggregation of child labour prevalence data for UN SDG regions. Where, NCL_i is the % of children in non-hazardous labour in country i, HCL_i is the % of children in hazardous labour in country i, and $OPCL_i$ is the country's overall prevalence of child labour.

$$NCL_i + HCL_i = OPCL_i$$

The generated overall child labour prevalence ($OCLP_i$) values are subsequently normalised using Equation 5-6. As seen with forced labour prevalence, this occurs on a max zero basis, both reversing directionality and ensuring a requirement of 0% child labour prevalence for a perfect score of 1.

Equation 5-6 – Normalisation of overall child labour prevalence (OPCL). Where, $OPCL_{Max}$ is the highest observed prevalence, $OPCL_i$ is the overall prevalence in country i, and $NCLP_i$ is the normalised prevalence of child labour for country i.

$$1 - \frac{OPCL_i}{OPCL_{Max}} = NPCL_i$$

With the normalised child labour prevalence ($NCLP_i$) determined for each UN SDG region, and thus their constituent countries, vulnerability can be incorporated. Vulnerability to child labour is not examined by the World Bank directly, necessitating a secondary data source. Consequently, the national vulnerability scores utilised within the forced labour CM (extracted from a WFF report [220]) are used as a proxy. Given a clear commonality in stimulating factors between forced and child labour [221], this is deemed a reasonable assumption. Incorporation of national level vulnerability as the second stimulating factor allows for upward or downward adjustment of the UN SDG region-oriented prevalence data, accounting for intra-region risk variations. The overall effect of this strategy is greatly improved geographic resolution. Using the previously processed WFF vulnerability data ($NVFL_i$), the final indicator value can be determined using Equation 5-7, delivering the national scoring profile for the G20 seen in Figure 5-4.

Equation 5-7 – Final indicator calculation for the risk of child labour. Where, $NPCL_i$ is the normalised prevalence of child labour in country i, and $NVFL_i$ is the normalised vulnerability to forced labour in country i.

$$0.5(NPCL_i + NVFL_i) = Risk\ of\ Child\ Labour$$

5.5.3 Risk of Change in Access to Electricity

In adherence to the methodological approach laid out earlier, literature was consulted to identify stimulating and de-stimulating factors with respect to energy access and security. Stavytskyy, *et al*. [222] present the only identified list of factors with a relevant scope, all of which are present within the World Bank database [223]. This includes;

- Renewable energy consumption (% of total final energy consumption) (De-stimulating factor)
- Energy Imports, net (% of energy use) (Stimulating factor)
- Electric power consumption (kWh per capita) (De-stimulating factor)
- Fossil fuel energy consumption (% of total) (Stimulating)

With the factors identified, their respective data sets are extracted directly from the World Bank. However, issues around data completeness are again encountered. Many countries show patchy reporting with no single year containing all required data across an acceptable number of countries. To circumvent this issue, the most recently available data is utilised in each case, generating a super-set (provided in the supplementary material). A hard limit on data age is implemented, backdating no more than ten years, preventing the incorporation of significantly aged data. This strategy results in complete data coverage for 142 countries, or 65% of those present in the database. Additional gaps cannot be filled without imputation.

Before normalisation of each factor, skewness is examined (using Equation 5-8) to identify any unintended implications of the temporally diverse data aggregation strategy. Through this, the skewness of electric power consumption data is revealed to be 4.74 (the only factor with a skewness >1). When using standard normalisation techniques, this significantly reduced the utility of collected data, tightly grouping a majority of countries with a few distant outliers. Furthermore, the raw energy consumption rate gives little insight to the more relevant per capita availability. Electric power consumption was therefore removed from further CM development.

Equation 5-8 – Method used for the calculation of data skewness. Where n is the sample size, x_i is the i^{th} value in the sample, $\bar{x}$ is the mean, and σ is the standard deviation.

$$skewness = \left(\frac{n}{(n-1)(n-2)}\right) \times \sum_{i=1}^{n} \left(\frac{x_i - \bar{x}}{\sigma}\right)^3$$

Renewable energy consumption (REC_i) is normalised on a zero to one basis (Equation 5-9) to deliver national scores reflecting their renewable grid shares ($NREC_i$), only awarding a perfect score to a 100% renewable grid mix. The upper bound observed within the data set is the Democratic Republic of the Congo, exhibiting a 96.24% renewable grid mix, a direct consequence of large hydroelectric and biogas capacities [224].

Equation 5-9 – Normalisation of national renewable energy consumption. Where, REC_i is the renewable energy consumption of country i (% of grid mix), and $NREC_i$ is the normalised renewable energy consumption of country i.

$$\frac{REC_i}{100} = NREC_i$$

Normalisation of net energy imports (NEI) is a more complex task, ultimately being handled by utility function (Equation 5-10). Many exporting countries exhibit highly negative values within this risk stimulating factor (e.g. Norway). These large-scale exporters introduce significant skew. Additionally, the export capacity of a country does not affect its own population's access to electricity, rendering its consideration moot. Consequently, any countries exhibiting negative NEI are assigned a value of one, attaining the highest possible normalised value ($NNEI_i$=1), signalling ideal performance. Conversely, a value of 100% import will receive a normalised score of zero, reflecting total dependence on non-domestic sources.

Equation 5-10 – Normalisation of net energy import (% of domestic use). Where, $NNEI_i$ is the normalised net energy import for country i, and NEI_i is the net energy import of country i.

$$NNEI_i = \begin{cases} 1 - \frac{NEI_i}{100}, & \text{for } 0 < NEI_i < 100 \\ 1, & \text{for } NEI_i \le 0 \end{cases}$$

The next stimulating factor identified is fossil fuel reliance (FER_i). The simplest of the normalisation cases, it is tackled on a max zero basis (Equation 5-11). Normalised scores fossil energy reliance ($NFER_i$) therefore delivers low scores for nations with high reliance, with high scores awarded for low reliance. This rationale, derived in conjunction with the work by Stavytskyy, *et al*. [222], reflects the uncertain energy futures of fossil reliant nations, owing to increasing fossil energy scarcity and tariffs.

Equation 5-11 – Calculation of normalised fossil energy reliance of country I ($NFER_i$). Where FERi is the fossil energy reliance of country i.

$$1 - \frac{FER_i}{100} = NFER_i$$

With the three contributing factors' scores normalised for all 142 available countries, aggregation into a final score is approached. Weightings are used, derived through practitioner judgement, delivering Equation 5-12. Normalised fossil energy reliance (NFER) is assigned the highest weighting (0.5), reflecting its notable influence on energy security in a world where fossil-based generation is being phased out. The resulting national scoring profile for the G20 is shown in Figure 5-5.

Equation 5-12 – Final indicator calculation for risk of change in access to electricity.

$$0.25(NREC_i + NNEI_i) + 0.5NFER_i = Risk\ of\ Change\ in\ Access\ to\ Electricity$$

5.5.4 Risk of Change in Access to Water

Access to water in the context of this work does not solely consider drinking water, instead examining access more broadly. This constitutes a challenge when identifying stimulating and de-stimulating factors, with the vast majority of literature focussing on rural access to drinking water [225] [226] [227]. Very little has been published in consideration of national-level water access. Therefore, an analogous approach is taken to that used for the risk of change in access to electricity. In this effort, the following factors are identified within the World Bank database, supplied by partner FAO AQUASTAT [228];

- Freshwater withdrawal as % of total renewable water resources (stimulating)
- Water Stress (%) (stimulating)
- Total renewable water resources per capita (m3/inhab/year) (destimulating)

Selected factors are chosen based on their alignment with the UN SDGs, primarily goal 6, and their focus on use as a function of national availability. Ultimately, there is a much lower risk of access reduction where the availability of renewable water resources is plentiful.

When examining each of the data sets, it was decided that total renewable water resources per capita should be excluded from the characterisation model, primarily owing to significant skew and co-linearity with freshwater withdrawal as % of total renewable water resources.

Smaller issues around skew were identified within the other two factors; however, they are eliminated through cut-off strategies. In this, any nation withdrawing more than 100% of its renewable water reserves is automatically considered to be at a maximum value of 100%. While this removes the ability to assess the negative impact of water imports, the dataset's skew is reduced from an unacceptably high value of 9.71 to an acceptable 1.86 (calculated using Equation 5-8). In this theme, the same approach is taken to water stress, capping reporting to a maximum value of 100%, again reducing the skew from 9.68 to 1.45. Overall, this strategy maintains reasonable bounds and skew in both cases. However, a small number of countries datapoints are artificially capped, totalling 12 for freshwater withdrawal and 17 for water stress; 90.4% and 93.2% of the 177 considered countries respectively.

Having resolved the problematic skewness and bounds, normalisation between limits of 0-100 is carried out for both freshwater withdrawals as % of total renewable water resources (Equation 5-13), and water stress (Equation 5-14) respectively.

Equation 5-13 - Normalisation of freshwater withdrawals as % of total renewable water resources. Where, $NRFW_i$ is the normalised renewable freshwater withdrawals for country i, and RFW_i is the renewable freshwater withdrawal of country i.

$$NRFW_i = \begin{cases} 1 - \frac{RFW_i}{100}, & \text{for } 0 < RFW_i < 100 \\ 0, & \text{for } RFW_i \geq 100 \end{cases}$$

Equation 5-14 - Normalisation of water stress. Where, $NNWS_i$ is the normalised national water stress for country i, and NWS_i is the water stress of country i.

$$NNWS_i = \begin{cases} 1 - \frac{NWS_i}{100}, & \text{for } 0 < NWS_i < 100 \\ 0, & \text{for } NWS_i \geq 100 \end{cases}$$

With these normalised values generated for the 177 considered countries, their aggregation is approached through an average (Equation 5-15). This gives the final national indicator scores for the risk of change in access to water.

Equation 5-15 – Final indicator score calculation for the risk of change in access to water.

$$0.5(NRFW_i + NNWS_i) = Risk\ of\ Change\ in\ Access\ to\ Water$$

5.5.5 Risk of Land Use Change

The potential risk of land use change was approached through the consideration of current land use proportions and the associated classifications. As per the overarching methodology, World Bank data is utilised directly to populate the inventory. National data was therefore extracted directly from the World Bank database to quantify the percentage of land mass occupied by agriculture, forest and protected land respectively. These areas are determined to be of the highest societal value and risk of repurposing, giving rise to the greatest potential for negative impact. It is considered that these areas are not necessarily mutually exclusive, instead harbouring potential overlaps, as indicated by Figure 5-2.

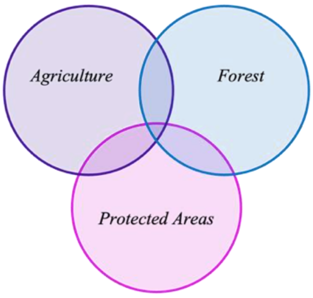


Figure 5-2 – Visualisation of the overlap of land area World Bank data within the categories of agricultural land, forest, and protected areas.

The inclusion of protected areas introduces the risk of double counting, potentially also being classified as areas of forest, or in current agricultural use. Examples of this can be seen within the U.K.'s New Forest National Park under the 'Farming in Protected Landscapes' grant programme [229], or the Wood Buffalo Protected Forest in Canada [230]. However, due to a lack of more granular and openly available data, these categories must be utilised in the most effective manner possible. In an idealised scenario, or future revisions, factors such as the availability of brownfield sites would also be incorporated into the CM.

When considering the sum of the three land classifications, the double counting becomes apparent, with four countries' values exceeding 100% of their land area: Micronesia (123%), Marshall Islands (119%), American Samoa (110%), and Sao Tome and Principe (105%). A further seven exhibit precisely 100%. A solution to the double counting issue is attained through the use of the larger value of either:

- Agriculture + Forest
- Protected areas

This method (expressed via Equation 5-16) is deemed acceptable in the absence of more robust and openly available data, delivering a lower bound for the nations denied land fraction (DLF_i).

Equation 5-16 – Calculation of denied land fraction (%) of country i (ALF_i).

$$DLF_i = \max\Big(\big(forest\ area\ (\%) + agricultural\ area\ (\%)\big) \vee \big(protected\ area\ (\%)\big)\Big)$$

With this lower bound of the denied land fraction quantified (DLF_i), the upper bound of each country's available land fraction (ALF_i) can be determined via Equation 5-17

Equation 5-17 – Determination of available land fraction of nation i (ALF_i) via the previously calculated denied land fraction of nation i (DLF_i)

$$1 - DLF_i = ALF_i$$

To account for disparities in population density, Equation 5-18 is employed. The result is an estimated upper bound for the available land per capita ($ALPC_i$) suitable for responsible development, offering a fair and comparable ranking metric.

Equation 5-18 – Calculation of available land area per capita for country i (ALC_i). Where, ALF_i is the assigned land fraction (%) of country i, NLA_i is the total national land area of country i, and p_i is the population of country i.

$$\frac{ALF_i \times NLA_i}{P_i} = ALPC_i$$

Having estimated the available land area per capita for the 204 countries with suitable World Bank data coverage, max zero normalisation is applied (Equation 5-19), revealing the normalised available land area per capita ($NALPC_i$). However, Greenland presents an outlier, returning an available land area per capita 18.36 times that of the second-highest score (Namibia); its consequential exclusion reduces the dataset's skew from 14.07 to a more acceptable but still highly significant 5.06 (using Equation 5-8).

Equation 5-19 – Calculation of the normalised available land area per capita for country i ($NALPC_i$). Where, $ALPC_i$ is the available land area per capita, and $ALPC_{Max}$ is the largest national available land area per capita.

$$\frac{ALPC_i}{ALPC_{Max}} = NALPC_i$$

While achieving normalised national scores, the observed skew of 5.06 is still significant, with a majority of values residing at the lower end of the range. To combat this, a utility curve is employed. After consideration of multiple exponents, 0.25 was ultimately selected (Equation 5-20). This is owing to the balance observed between additional resolution achieved at the lower values, while maintaining a slight skew to reflect the original data character. It is recognised that the selection of the exponent is, to some extent, subjective. However, when communicated transparently, this is deemed acceptable in the interest of heightened utility to practitioners and assessments. The results of the CM for the G20 countries can be seen in Figure 5-7.

Equation 5-20 – Calculation of the risk of land use change indicator score. Where, ($NALC_i$) is the normalised available land area per capita for country i

$$NALC_i^{\ 0.25} = Risk\ of\ Land\ Use\ Change$$

5.5.6 Occupational Safety & Health

Occupational safety and health (OSH) represents a common impact category within SIA. Typically, this is assessed using primary data from the process of interest. However, in the pre-deployment setting of this research, no primary data will be available. Additional complexity is encountered in the lack of OSH data available through the World Bank. Several alternative data sources were considered, with many offering poor coverage (e.g. only 96 countries from ILOSTAT) [231] [232]. Suitable alternative data was identified, through a World Bank partner; ILO's summary of work-related mortality [233].

This ILO data exhibits excellent coverage with 216 countries fully defined. However, its age is less than optimal, hailing from 2003. With the search for more recent literature returning nothing of note, progression based on legacy data must be accepted. This requires the assumption that the rate of workplace injuries and illnesses have remained largely proportional across the examined countries and temporal shift, constituting a current limitation and opportunity for future development.

Through this ILO data, the following stimulating factors are extracted at the national level [233, 233];

- Accidents causing four days of absence (Stimulating)
- Work-related disease (Stimulating)
- Work-related mortality (Stimulating)

Data processing is required to allow for fair comparison between countries for each factor. To this end, accidents causing four days of absence, work-related disease, and work-related mortality are converted to occurrence rates by dividing by the national economically active population as provided within ILO's data (per 10,000 workers). These occurrence rates are then normalised (max zero) and corrected for directionality using Equation 5-21, Equation 5-22, and Equation 5-23.

Equation 5-21 – Calculation of normalised occurance rate of accident related absence per capita ($NORA_i$). Where, ORA_i is the occurance rate of accident related absence for country i, and ORA_{Max} is the maximum value observed for occurrence rate of accident related absence across all countries.

$$1 - \frac{ORA_i}{ORA_{Max}} = NORA_i$$

Equation 5-22 – Calculation of normalised occurance rate of work related disease per capita ($NORD_i$). Where, ORD_i is the occurance rate of work related disease for country i, and ORD_{Max} is the maximum value observed for occurrence rate of non-fatal accidents across all countries.

$$1 - \frac{ORD_i}{ORD_{Max}} = NORD_i$$

Equation 5-23 – Calculation of normalised occurance rate of fatal accidents per capita ($NORF_i$). Where, ORF_i is the occurance rate of fatal accidents for country i, and ORF_{Max} is the maximum value observed for occurrence rate of fatal accidents across all countries.

$$1 - \frac{ORF_i}{ORF_{Max}} = NORF_i$$

This delivers normalised national scores between 0-1 (higher scores being preferable) for each stimulating factor. For the characterisation of each country's OSH performance, the three factors are assigned equal weightings, resulting in Equation 5-24. The final national scores for the G20 countries can be seen in Figure 5-8.

Equation 5-24 – Aggregation of the stimulating factors contributing to OSH indicator scoring.

$$\frac{1}{3}(NORA_i + NORD_i + NORF_i) = Occupational\ Safety\ and\ Health\ Indicator\ Score$$

5.5.7 Risk from Utilization of Hazardous Materials

Characterisation of risk from the use of hazardous materials is challenging, a consequence of its heavier dependence on the industrial sector than the country of deployment. Aggravating this, data is severely lacking. It is proposed that the risk from the use of hazardous material should be represented through its impacts rather than raw prevalence in a supply chain. Where these materials are handled well, under properly enforced and effective regulations that result in no negative impact, the value chain should not be penalised.

An idealised characterisation approach would include a breakdown of fatal and non-fatal incidents caused by the industrial use of hazardous materials within each sector and country. However, this scenario is far from being realised. Furthermore, the World Bank does not provide any datasets suitable for use as stimulating or de-stimulating factors. In the absence of such data, an alternate approach is required. The ILO provides data on the number of work-related deaths from exposure to hazardous materials (WDHS) in each nation's economically active population (EAP) [233]. Equation 5-25 delivers a national-level value for work-related deaths from exposure to hazardous materials per 10,000 workers.

Equation 5-25 – Calculation of the risk of death from exposure to hazardous substances for country i ($RDHS_i$), Where, $WDHS_i$ is the workplace deaths from exposure to hazardous substances for country i, and EAP_i is the economically active population of country i.

$$\frac{WDHS_i}{EAP_i} \times 10{,}000 = RDHS_i$$

With these risk values determined, normalisation can be carried out (Equation 5-26) relative to the set's maximum value. Directionality is also reversed to deliver a higher score for lower risk. The resulting national scores for the G20 (excluding the African & European Unions) can be seen in Figure 5-9 (full list of national scores available in ESI).

Equation 5-26 – Calculation of the risk from the utilisation of hazardous materials in country i ($RUHM_i$). Where, $RDHS_i$ is the risk of death from exposure to hazardous substances for country i, and $RDHS_{Max}$ is the highest observed risk of death from exposure to hazardous substances.

$$1 - \frac{RDHS_i}{RDHS_{Max}} = RUHM_i$$

5.6 Results

Overall, the seven indicators examined within this study show that it is possible to derive impact pathway-based SIA CMs analogous to those observed in LCA. However, data reporting and, therefore, availability is easily identified as the limiting factor. The results of the CMs developed can be seen in Figure 5-3 to Figure 5-9; for ease of interpretation, only the G20 countries are shown (excluding the African and European Unions), and the full data set, including all 239 examined countries, and the underpinning literature data, is available in the electronic supplementary material (ESI).

The developed SIA CMs exceeded initial ambitions concerning coverage. However, this coverage was, in places, achieved through slight methodological compromise (e.g. risk of land use change and risk from utilisation of hazardous materials). Good geographical coverage is essential to the development of SIA CMs; a perfectly defined impact pathway model is of no practical use if it relies on unavailable input data. In total, 239 countries are listed by the World Bank data sets [234]. Of these, 129 countries are fully defined (~54%), with a further 32 (~13%) missing only one single data point. Completeness of coverage is detailed in Table 5-2.

Table 5-2 - Model coverage based on the number of indicators fully characterised per nation.

Number of Indicators Fully Defined	Country Count
7	129
6	32
5	17
4	33
3	1
2	25
1	2
TOTAL	239

These calculations reveal that most indicator scoring profiles (four of seven) exhibit a mean value of 0.5±0.1, the midpoint of the normalisation scale. These are: the risk of child labour, risk of change in access to electricity, occupational safety and health, and utilisation of hazardous materials.

Further examination shows that of these four indicators, occupational safety and health, and utilisation of hazardous materials exhibit significant skew (-1.3934 and -1.8647, respectively). In both cases, this can be attributed to very low scores for African nations. While a statistically significant skew, this is not considered a methodological shortcoming. Instead, it reveals markedly poor national performance relative to the global averages. Compounding this, a correlation between these indicators is expected. When these final indicator scores are paired for each country, a correlation of 0.9229 is observed (ref. Table 5-4), verifying the previous assumption.

In contrast, three indicators show mean scores with significant deviation from the midpoint: risk of forced labour (0.7408), risk of change in access to water (0.7699), and risk of land use change (0.3444). Of these, only the risk of forced labour has an insignificant skew, indicating generally high scores for most nations. This is attributed to two factors: relatively low average national prevalence, and significantly elevated national prevalence in the DPRK (resulting in a slightly outlying lower bound for normalisation). The other two cases of deviated means (risk of change in access to water and risk of land use change) can be explained by regional concentrations within risk and security profiles, producing sets of geographically related outlying nations. In the case of risk of change in access to water, this is attributed to elevated water supply risk in the Middle East, confirmed by the CM results in Figure 5-6 and the ESI. The deviated mean value for land use change, delivering typically low national scores, is attributed to very low risk (high scores) in countries with sparse populations (e.g. Greenland, Iceland, and Australia).

Collinearity of national indicator rankings is characterised within Table 5-4, allowing for the identification of potentially related social impacts. Where high collinearity is identified, the utility of assessing both indicators may be reduced, helping practitioners and stakeholders to streamline an assessment's goal and scope. Several indicator pairs exhibit a strong correlation: risk of forced labour and risk of child labour (0.7259), risk of child labour and OSH (0.7609), and OSH and utilisation of hazardous materials (0.9229). While an interesting insight into inter-indicator causal relationships, this alone should not independently drive the omission of an indicator if it is highly relevant to the scope of the SIA. However, it may aid the selection of indicators in time-constrained or screening assessments.

Examining the national scores across the CMs developed, some intriguing findings are revealed. For example, the CM for risk of access to electricity prescribes the highest overall score to the Democratic People's Republic of the Congo (0.9674). Since 2012, the country has had a relatively stable, forward-looking, 99% renewable electricity mix, with 96% of this being hydroelectric (Inga I and Inga II dams) [235] [236], supporting the result.

When examining OSH, many of the highest-scoring nations are micronations, such as Nauru, Tokelau and Turks and Caicos (scores detailed within the supplementary material). These high scores are explained by their import of many goods produced through hazardous industries, themselves lacking the resources or demand to support domestic operations. However, the scope of this assessment focuses on value chains. Consequently, any assessment of goods derived through hazardous industry would include the producing country, not simply the country in which the point of sale or end-use resides. For this reason, the highly positive scores for micronations are deemed accurate.

Table 5-3 - Mean and skewness values for the derived SIA indicator CM data sets.

SIA Indicator	Mean National Score	Skew	Standard Deviation
Risk of Forced Labour	0.7408	-0.8748	0.1387
Risk of Child Labour	0.5561	-0.4756	0.2551
Risk of Change in Access to Electricity	0.4877	-0.1173	0.2292
Risk of Change in Access to Water	0.7699	-1.5603	0.3036
Risk of Land Use Change	0.3444	1.3387	0.1676
Occupational Safety and Health (OSH)	0.5780	-1.3934	0.1844
Risk from utilisation of Hazardous Materials	0.5999	-1.8647	0.2127

Table 5-4 - Collinearity between national indicator scores. These values only include the 129 countries for which all seven indicators are fully defined. Green denotes high collinearity, with red indicating low collinearity.

	Risk of Forced Labour	Risk of Child Labour	Risk of Change in Access to Electricity	Risk of Change in Access to Water	Risk of Land Use Change	Occupational Safety and Health (OSH)	Risk from utilisation of Hazardous Materials
Risk of Forced Labour	1						
Risk of Child Labour	0.7259	1					
Risk of Change in Access to Electricity	-0.3785	-0.4932	1				
Risk of Change in Access to Water	0.1965	0.0528	0.2360	1			
Risk of Land Use Change	0.0072	0.0232	0.1482	-0.0993	1		
Occupational Safety and Health (OSH)	0.4225	0.7609	-0.5255	-0.3091	-0.0120	1	
Risk from utilisation of Hazardous Materials	0.2185	0.5662	-0.3944	-0.2945	-0.0626	0.9229	1

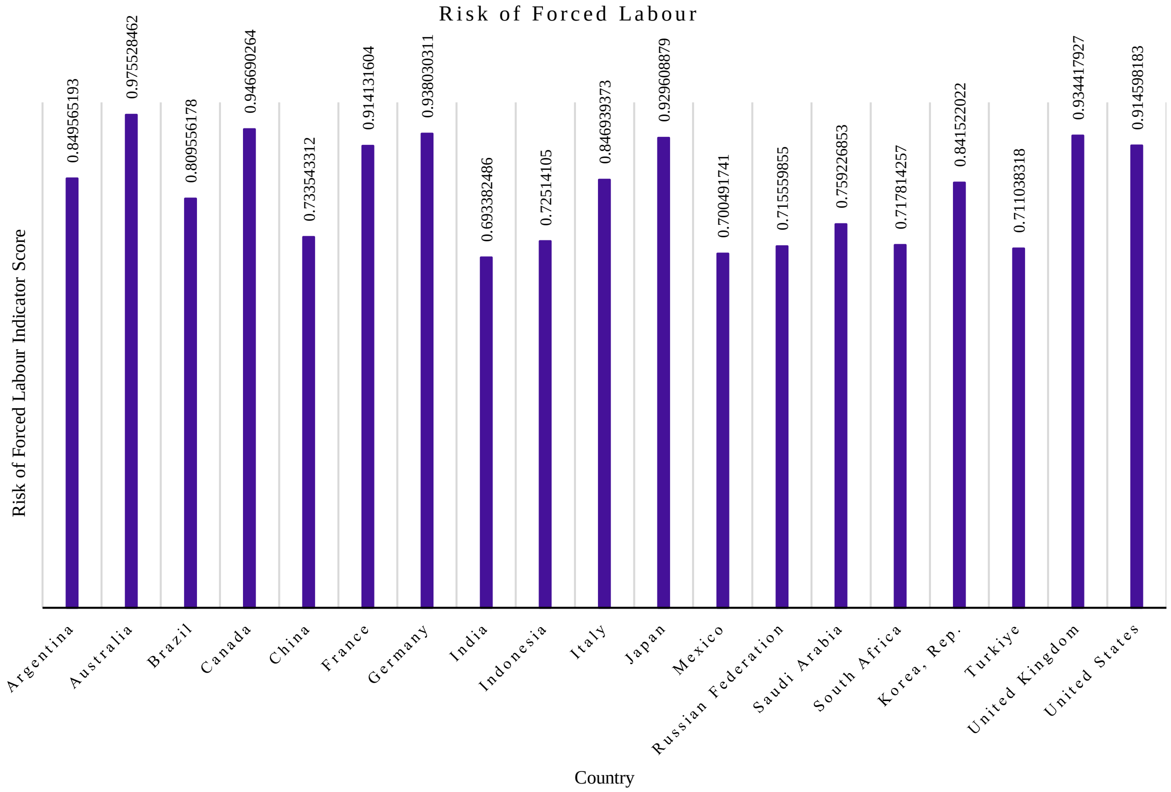


Figure 5-3 - Forced labour indicator results

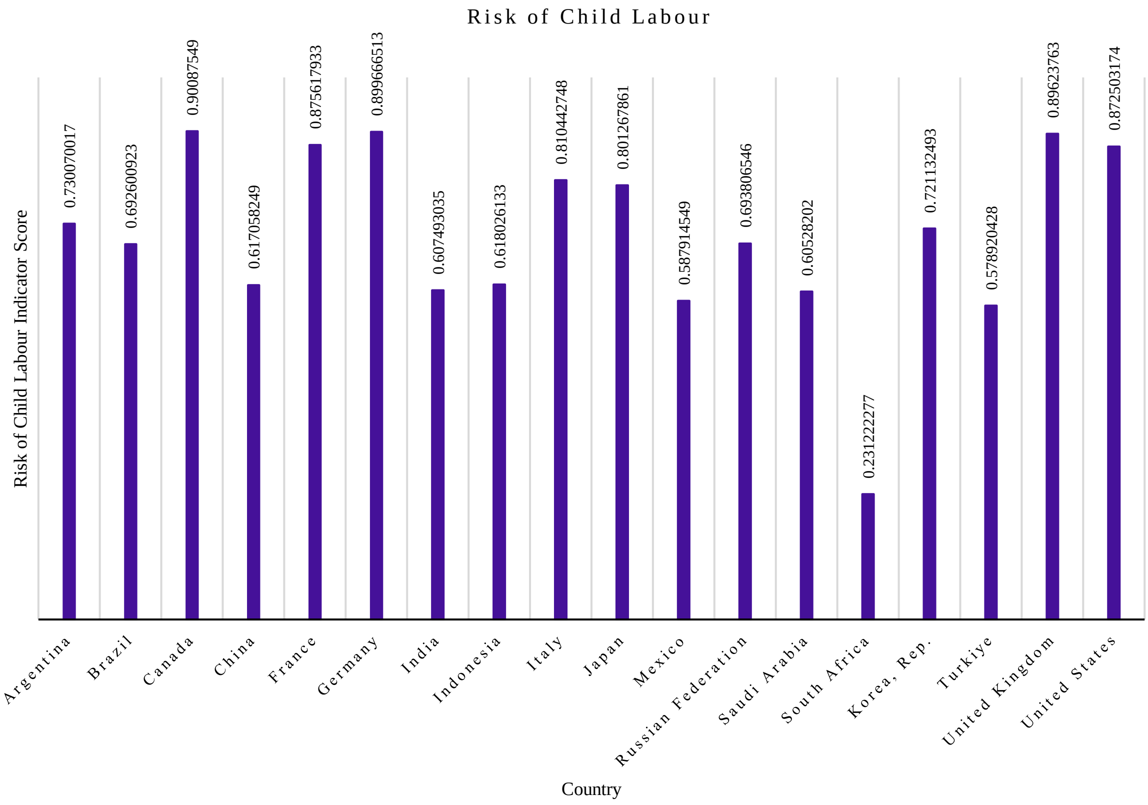


Figure 5-4 - Child labour indicator results

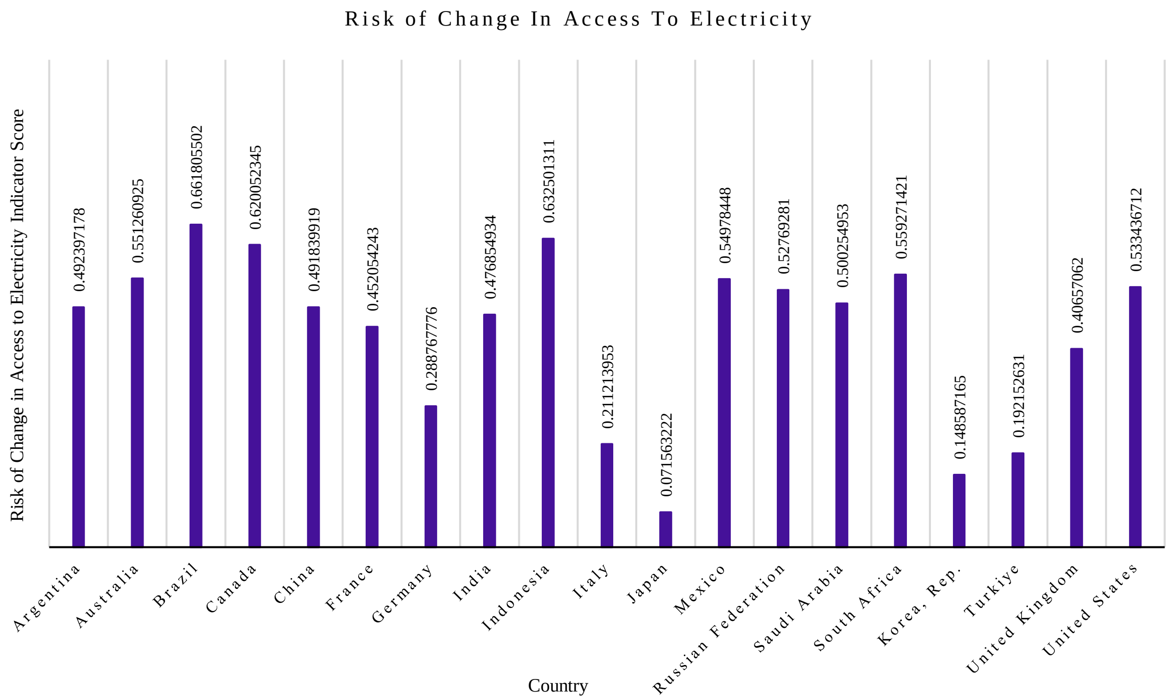


Figure 5-5 - Access to electricity indicator results

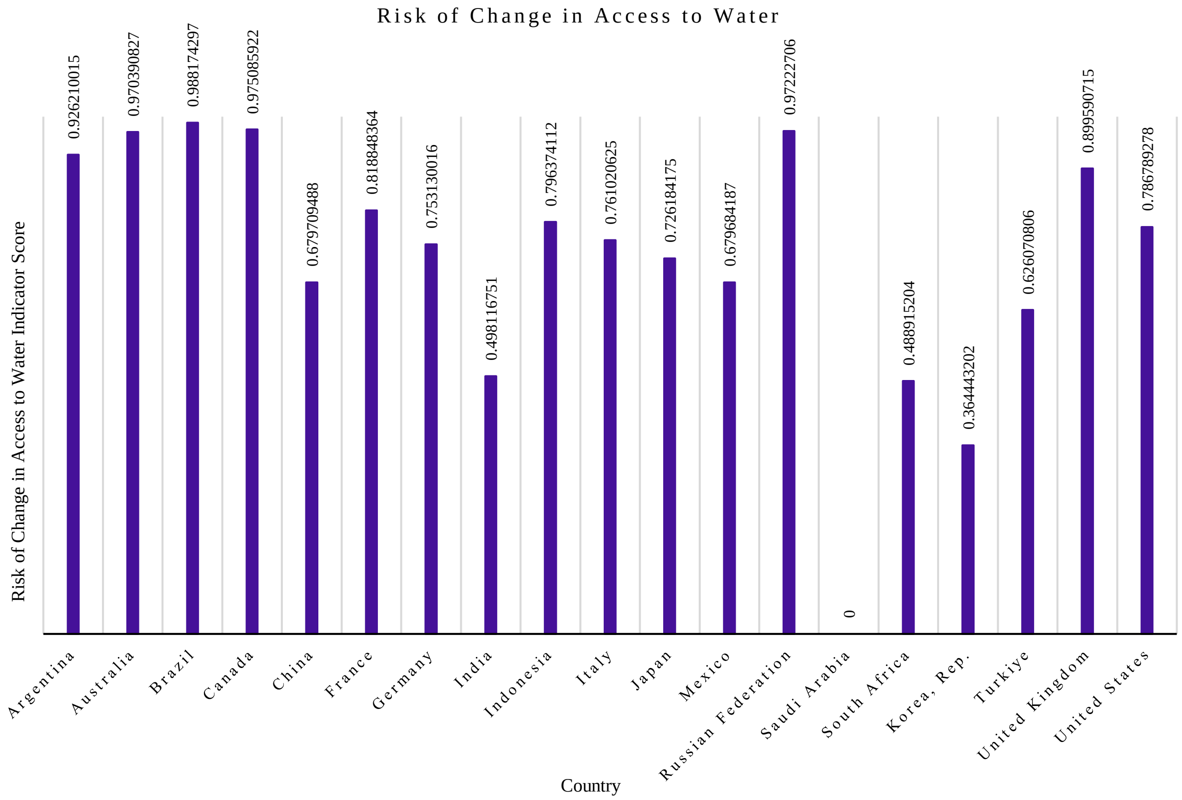


Figure 5-6 - Access to water indicator results

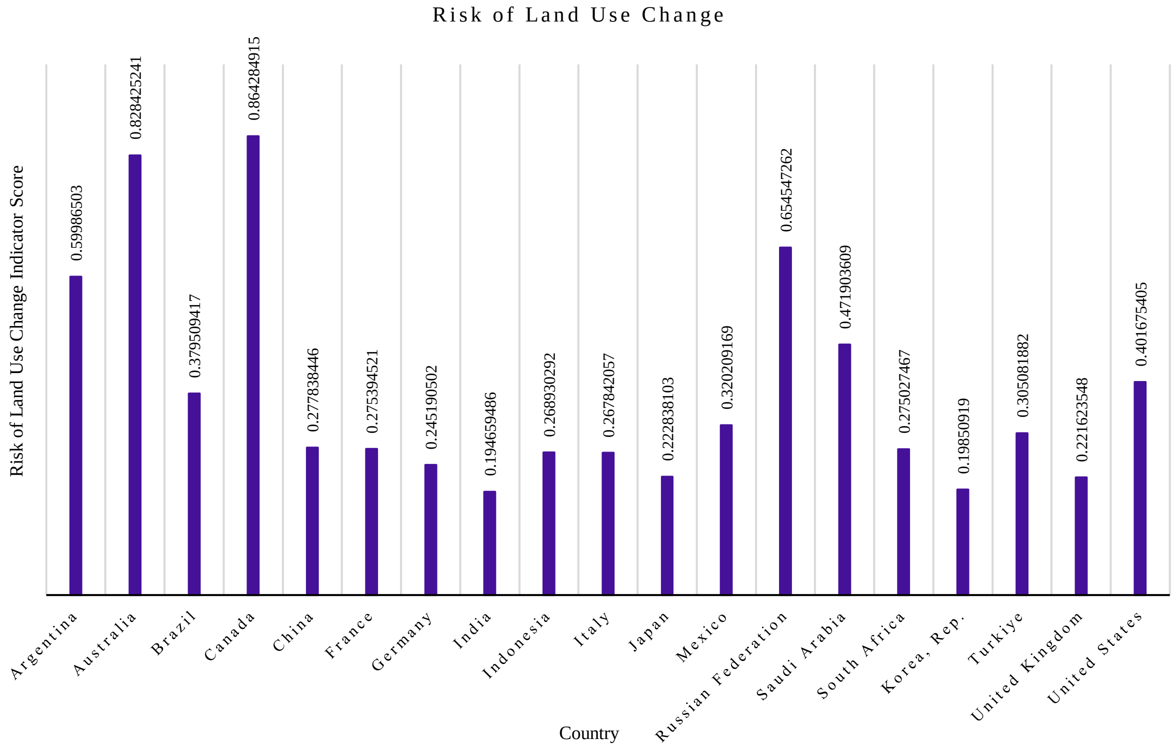


Figure 5-7 - Land use change indicator results

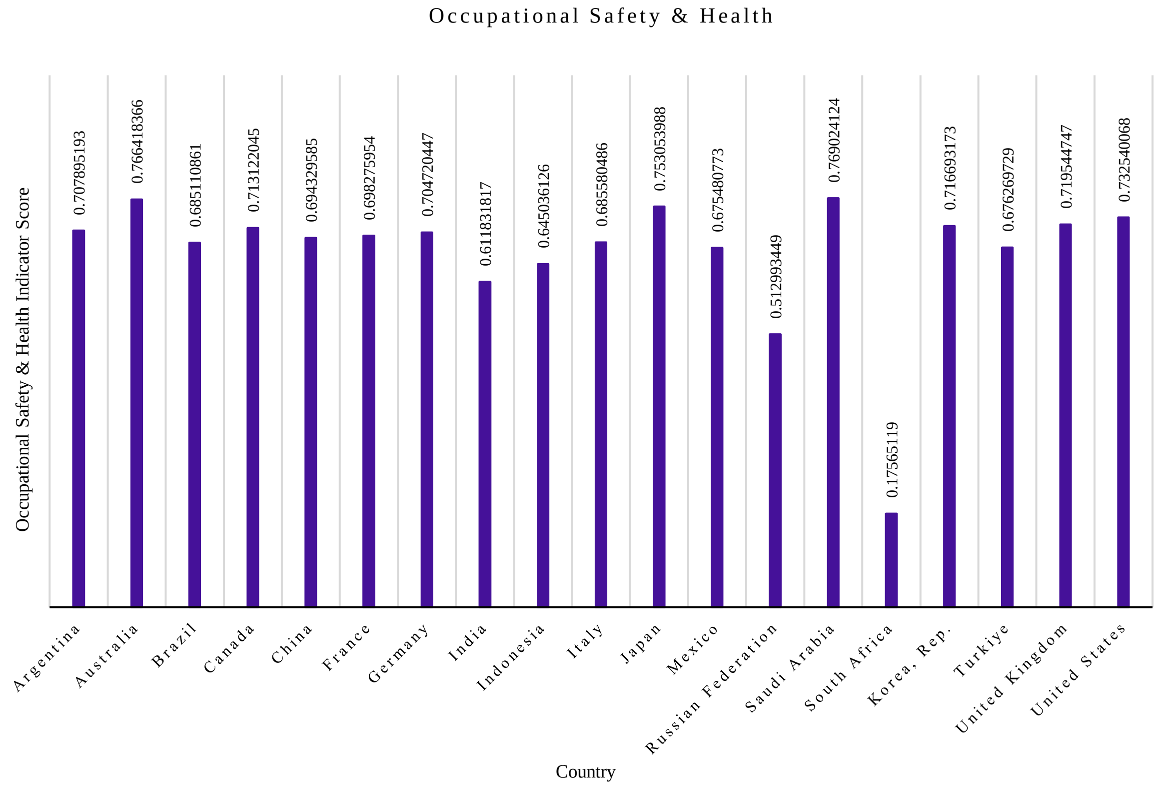


Figure 5-8 - Occupational health and safety indicator results

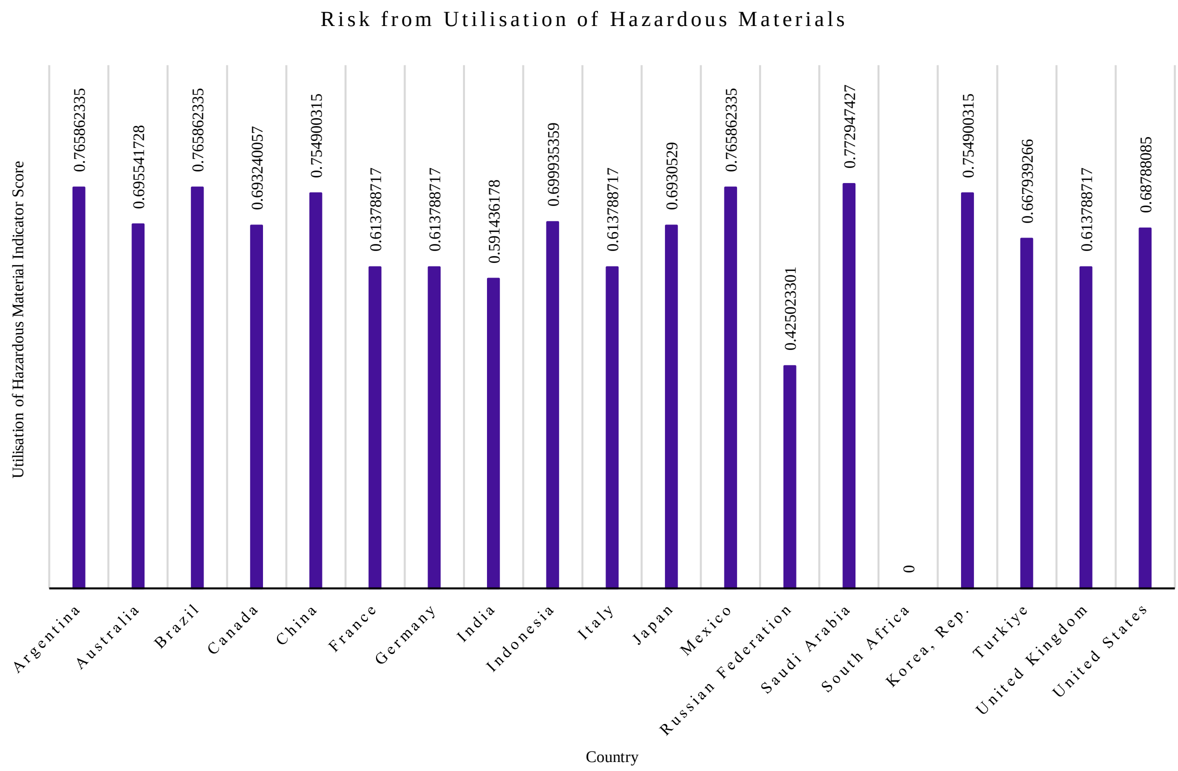


Figure 5-9 - Utilisation of hazardous material indicator results

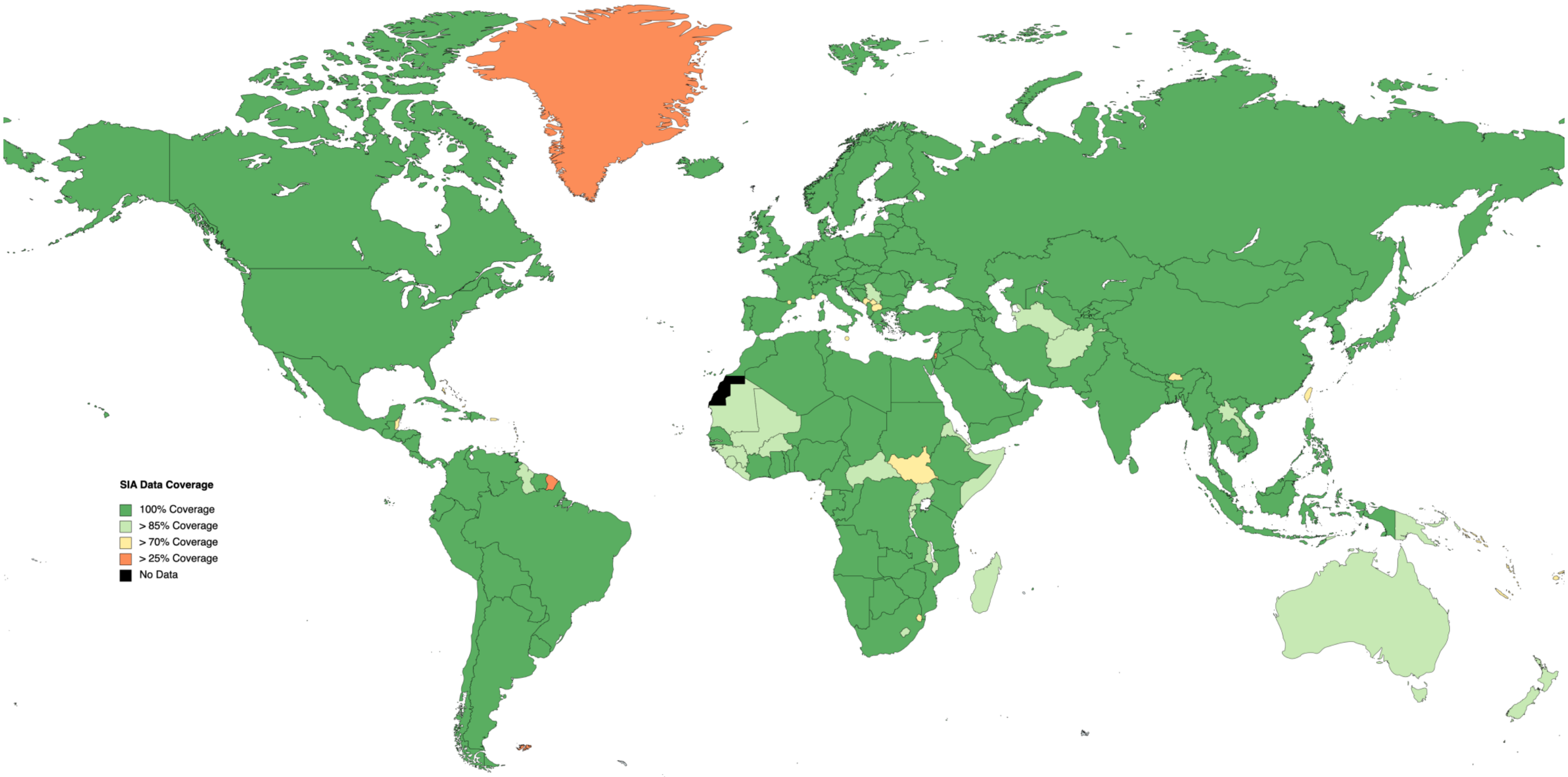


Figure 5-10 - SIA characterisation model coverage map

5.7 Discussion

This work represents a first step towards value chain-oriented impact pathway SIA CMs, delivering a novel development in the pursuit of harmonised holistic sustainability assessment. Previously, reference scale approaches have dominated within parallel lifecycle, techno-economic and social sustainability assessments [7]. This bifurcation in impact characterisation methods has been identified in previous literature as a barrier to fully integrated studies [200]. Through the this set of initial impact pathway SIA CMs , the difficulties surrounding the integration of SIAs to holistic assessments are partially rectified, most notably the subjectivity and reliance on practitioner judgment observed within previous reference scale approaches.

Methodologically, the seven selected indicators follow similar approaches, each utilising open literature to examine appropriate stimulating and de-stimulating factors. They are then aggregated using specified formulae. These are derived to both effectively utilise the collected data, and to normalise national scores. However, in the cases of risk of change in access to electricity and risk of change in access to water, significant skew (up to a magnitude of 14.07) can be seen in the data sets of the stimulating and de-stimulating factors. Causation can be traced to the presence of extreme outlier countries. These are systematically removed by the specification of artificial normalisation boundaries. Through this, outlier scores are assigned a normalised value of either one or zero, depending on the direction in which they exceed the boundaries. Failure to remedy such extreme skews would lead to either a dampened or amplified contribution of the factor to the overall aggregated indicator scores. Positive skews lead to dominant factor behaviour, whereas negative skews deliver recessive behaviour. Through the use of the mentioned artificial normalisation boundaries, all indicators exhibit final skews of $< |2|$. While a magnitude of 2 is highly significant, the aim is not to remove all skew; such data character is often representative of real-life performance differentials. Consequently, a balance must be struck to deliver meaningful national indicator score profiles while still representing real performance (including a degree of skewness).

Examination of collinearity between indicators (Table 5-4) shows some strong links; for example, a correlation coefficient of 0.9229 for OSH and utilisation of hazardous materials. While these are not unexpected, it does raise interesting questions around the selection of indicators. Should strongly colinear indicators be assessed within the same study, or can their correlations be used to evaluate factors vicariously? Ultimately, this should depend on the goal and scopes of specific CM applications.

Several objectives, or requirements, of the CMs were detailed in the introduction. These were specified to ensure relevance to the development of novel CDU value chains and included; applicability to a wide range of TRLs and technology types, assessment of pre-deployment scenarios, reliance on open-source data, and a national level geographic resolution. Each of these is discussed, determining the degree of attainment realised.

The development of CDU oriented value chains, an unavoidable challenge if such processes are to be commercialised at meaningful scale, must often occur in the absence of primary or deployed data. By adopting a red-flag approach, and removing all reliance on primary process data, the CM procedures are successfully aligned with the evaluation of CDU projects. Simultaneously, this avoidance of primary data delivers the desired applicability to the broad TRL range observed in CDU technologies. Consequently, a 'level playing field' is attained, upon which overly cautious or optimistic low TRL CDU processes do not receive an undue data-induced penalty or advantage. Such comparative assessments of CDU projects were previously identified in literature as lacking [39, 7], directly highlighting the utility and value addition of the developed CMs.

The requirement to use methodologically prescribed, and open source, databases (primarily the World Bank) delivers greater assessment transparency to all stakeholders. If all assessments were to utilise the same impact pathway reporting methods and metrics, issues around comparability (as mentioned by Zimmermann & Schomäcker [45] in the context of CDU TEA) would be significantly reduced. The World Bank is also utilised as a primary data source within the PSILCA v.3 methodology [237], aligning this work's approach to that of methodologies examining deployed systems. Furthermore, the use of the World Bank database facilitates the incorporation of temporal updates, allowing the CMs to reflect ongoing progress or regression at the national level. In effect, the ranking order of countries against a given indicator becomes temporally dynamic, mirroring reality through the incorporated range of real-world stimulating and de-stimulating factors.

Having identified early in the paper that the pre-deployment state of many CDU projects necessitates impact risk characterisation on a national level, data is extracted from the World Bank and applied through the CMs on this basis. Examination of Table 5-2 shows that 129 countries, a majority of those listed by the World Bank (53%), are fully defined across all seven indicators. Many more (32 countries, or 29% of those not fully defined) require remedial action over only a single data point. In total, only 12% of nations realise coverage in less than half of the indicators. Additionally, most countries exhibiting data gaps are, in terms of land area, very small, or lack unanimous international recognition (e.g. Taiwan). It is proposed that imputation be used to remedy these issues where necessary, manually filling the identified data gaps. However, this practice requires care in order to select meaningful proxy values. Implemented procedures should involve the use of data from an analogous nation, with fitness being based on both the country's GDP per capita and geographic proximity. A more simplistic approach, such as the use of a neighbouring country's data, can lead to inaccuracies stemming from factors such as incongruent socioeconomic profiles or the State's public spending capacity (e.g. PDRK and S. Korea). In addition, where this is carried out, resulting studies should acknowledge the use of proxy data and transparently communicate the nature of any remedial action taken.

The most notable data coverage issues occur where performance metrics are evaluated as an average for large geographic areas, hampering granularity. National-level data is far more valuable to an assessment practitioner than continental. The only encountered example of continent-based reporting can be seen in UNICEF's child labour prevalence figures; the report also omits Oceania [221]. In this specific case, the strong correlation between causal factors of both forced and child labour permitted the augmentation of scores using the WFF's vulnerability score. This effectively tunes the national performances within each UN SDG region, delivering a more representative and granular indicator score. Despite the positive impacts of this strategy, ideally, it will be superseded in the future by national child labour data.

Through these incorporated attributes the methods developed are seen to be highly applicable in the context of CDU value chains, catering to all of the identified nuances and difficulties. It should be recognised that these CMs are less granular than LCA CMs, and potentially the PSILCA database; however, this is currently unavoidable in the evaluated context (extensive TRL range and pre-deployment nature). It is proposed that once CDU as a field reaches maturity and widespread deployment, more generically applicable SIA approaches can be taken. However, the application of impact pathway-based methods should be proliferated in favour of reference scales.

As demonstrated, impact pathway assessments offer significantly enhanced repeatability when compared to their reference scale counterparts, circumventing the utilisation of practitioner judgement. Using relevant quantitative data and clearly specified calculation procedures, the delivered CMs are highly comparable to those of LCA and TEA, with the only major deviation being the previously noted geographic granularity. Consequently, any practitioner, irrespective of experience or background, should derive identical indicator results for the same system and assessment boundary. This is one of the cornerstone values of LCA and TEA CMs and should be adopted more comprehensively within SIA. In contrast, the reference scale approach's reliance on the practitioner's placement of alternatives on statement or criteria-based incremental scales, invites subjectivity and bias while simultaneously delivering less accountability or justification.

Such benefits to CDU oriented assessments are, however, achieved at the expense of other aspects. These include but are not limited to local reporting completeness and practices, quantifying the effectiveness of remedial actions, and perturbations in geopolitical stability. To fully understand the net scientific value addition delivered by the proposed CMs, these factors must be explored, and their implications clearly communicated.

The utility of, and confidence in, the generated indicator results would benefit significantly from the inclusion of data quality metrics. It is a reasonable assumption that less industrially and economically developed nations will have less reliable and transparent reporting practices around some indicators (e.g. the utilisation of hazardous materials and occupational safety and health). In countries and indicators where reporting practices for negatively impactful incidents are believed to be questionable, under reporting of risk is likely to occur. Robust quantification of such reporting quality is currently absent from the employed literature, making this shortcoming difficult to rectify. However, it should be incorporated as a measure of uncertainty in the generated result if or when it is available.

Some of the assessed indicators also lack valuable stimulating and de-stimulating factors due to their absence from open-source data. Key examples include the percentage of the population with access to reliable water and electricity. While such information is partially available, covering specific countries within isolated assessments, a consistent calculation method and broad coverage remain elusive. Aggregation of data from independent assessments would result in an unreliable and incomparable inventory, even in cases where full geographical coverage can be achieved. If a levelized quantification procedure and results are made available for these factors in literature, their integration would significantly augment the insights generated through the CMs.

Despite the CM's delivery of quantified indicator results, this does not in itself help organisations to mitigate the risk of negative social impact hotspots. As a red-flag risk-based assessment, this is expected. Direct resolution strategies can realistically only be identified in assessments of deployed activities. While this represents a limit of the study, it is one that will unavoidably impact all pre-deployment assessment methodologies equally. Instead, it is suggested that maximum utility is extracted from the CMs by using it to focus monitoring and mitigation efforts during the deployment phase on areas identified as high risk. This will allow the operating organisation to plan and optimise CDU value chains around these high-risk areas, hopefully reducing the final deployed impacts.

Practitioners should also note that on occasion the red flag based approach leaves gaps in impact characterisation coverage, an unavoidable consequence of the available data resolution. A pertinent example of this can be seen within the risk of change in access to electricity indicator; here, characterisation is based on examination of renewable share of grid mix, net energy imports, and fossil energy dependence. While for a majority of cases this provides a good indication of the population's electrical energy security, it does not account for reliability or coverage of distribution infrastructure. The impact of this can be seen clearly in the result generated for the Democratic Republic of the Congo, with its large renewable grid shares and low dependence on energy imports leading to a positive performance in the indicator. However, in this case, acceptance of the indicator result at face value risks omitting the detrimental effects of the country's poor distribution coverage and capacity. In reality, this limits per capita access to the generated electricity energy, instead favouring industrial users [224]. The opposite effect may also occur in countries where efficient and reliable distribution is present, more effectively delivering reliable access to electricity throughout the population despite smaller domestic generation capacities. Consequently, when evaluating deployment opportunities in developing or geo-politically unstable countries, organisations should utilise the presented characterisation models with caution, exercising additional due diligence around the just use of distribution infrastructure.

As touch upon briefly during the discussion of access to electricity, geopolitical stability, or lack thereof, is source of general inaccuracy within all SIA approaches. All organisations, including those targeting the deployment of CDU technologies, are facing more frequent and severe geopolitical events [238]. Such incidents can significantly elevate the risks of negative social impact. While not typically a consequence of the operating organisations actions, the accuracy of results is clearly impacted. Where this issue is observed, it is expected that the organisation would already be suspending deployment, or at the very least exercising additional due diligence. In light of this fact, and the case specific nature of such issues ,they are not targeted for resolution.

As noted in the literature review, there are several philosophical commonalities between this work and the PSILCA database approaches. The similarities and differences must therefore be assessed from a methodological stance by consulting the PSILCA database's documentation [214]; a quantified results-based comparison would require conduction of an applied case study and access to the paywall protected database. Recognising this, the seven developed indicator calculation procedures have been compared to their PSILCA counterparts. Initially, it is noticed that several indicators do not have a PSILCA equivalent and therefore cannot be compared: access to electricity, risk of land use change, and utilisation of hazardous material. Additionally, within PSILCA, reporting is not carried out on a comparable numerical basis. Instead, the indicators have their own quantified scoring approach which is then transposed to a risk-based reference scale (e.g. no risk, very low risk, low risk, etc.). Through this, the methodologies presented in this paper offer more easily interpreted results and, overall, a greater degree of granularity through the avoidance of reference scales.

Beyond these cases, subtle but notable divergences in methods can be observed. The most notable case is seen in the child labour indicator. Where the approach developed in this work examines both prevalence and future vulnerability, the PSILCA database focuses on purely prevalence; inclusion of future vulnerability represents a significant additional insight. Furthermore, the threshold for what constitutes child labour is lower within PSILCA's offering, including anything above one hour of economic activity per week as child labour. In contrast, the proposed methodology uses the UNICEF definition (see Figure 5-1) with more nuanced categorisation considering aspects such as hazard level.

Forced labour is considered on a broader basis within PSILCA than this paper's methodology, incorporating debt bondage, forced marriage, and child labour within the impact characterisation. While this expands coverage, there is discussion to be had around whether these impact mechanisms should fall under the umbrella of forced labour, or if they deserve consideration within their own indicator. At their cores, the two methods are procedurally very similar, both utilising the Global Slavery Index as an initial data source.

Access to water is approached from opposing classification ideologies. Where PSILCA evaluates access to drinking water, the methodology developed in this work looks at the more general availability of water as a resource. The PSILCA approach examines the local proximity of potable water sources to domestic dwellings, while generating high resolution insights, the approach conflicts with the lack of geographic specificity often surrounding CDU projects.

Finally, the occupational safety and health indicator (referred to as health and safety within PSILCA) is handled very similarly within the two methodologies. The primary differentiator is aggregation. Within this paper the non-fatal and fatal accidents are normalised, and the two values averaged to deliver a single indicator value. In contrast, PSILCA reports the two scores independently. While granularity is improved through PSILCA's approach, this brings with it difficulties in balancing trade-offs between the two values. Utilisation of the same data sets ensures highly comparable results between the two methods.

It is proposed that practitioners exercise the social impact characterisation methods developed within this work within holistic assessments of pre-deployment or scoping projects, particularly those with a CDU focus. Given this methodology's national level approach to impact characterisation, alternatives such as UNEP and SETAC's guidelines are often better suited to the assessment of deployed projects; despite utilising a more subjective reference approach, they are able to better capture site specific nuances.

Within holistic evaluation of pre-deployment CDU projects, it is suggested that the results of the LCA and TEA assessment strands are utilised as a first screening step, removing any alternatives with impacts exceeding acceptable thresholds in these areas. Subsequently, the revised list of competing options should be evaluated against the social impact indicators using the developed characterisation methods, identifying any hot spots representing elevated risk. These highlighted sources of potential impacts (e.g. risk of access to electricity within countries with small, weak or intermittent distribution grids) should then be used to indicate areas where elevated due diligence is required at the point of deployment, mitigating risks at their source to prevent negative social impacts from occurring. In the example of a project looking to deploy an energy intensive process in a country with poor electricity infrastructure, the associated risk hotspot may be remedied through the inclusion of on-site generation such as a CHP plant. This modification to the project would ensure that no negative social impacts are caused in terms of local communities' access to electricity; however, would require another iteration of the LCA and TEA results to ensure no significant burden shifting occurs.

Future work in the area should include the identification of a quantified indicator score threshold, below which a clear red flag is raised, indicating an elevated duty to due diligence. This would allow for clear and consistent communication of results to non-practitioners. Furthermore, such a standardised approach would remove the dependency of hotpot identification on less repeatable practitioner judgment. Remedial approaches may adopt a relative scale, flagging results below an n^{th} percentile of national scores. Alternatively, an absolute threshold may be specified (the more likely solution), removing the potential for misleading results within indicators exhibiting significant data skewness.

Sensitivity analysis around the weighting of each CM's stimulating and restimulating factors would also add significant value. Furthering understanding around the factor's relationships and influence on national rankings. Such work may inform a future revision of weightings.

A final obvious avenue for development is the development of CMs for additional indicators. As an initial proof of concept, this work only tackles a sub-set of UNEP and SETAC's noted impact sub-categories. To achieve broader applicability to a diverse range of goals and scopes, the current set must be expanded relatively significantly. Once completed, a full foundation will have been constructed for future impact pathway-based screening SIAs.

5.8 Conclusion

In conclusion, this proof-of-concept exercise has successfully demonstrated the utility of impact pathway SIA CMs in the context of CDU value chain development, while also realising applicability to more general use cases. The nuances of application scenarios, usually including integration with LCA and TEA, significantly reduce the effectiveness of previous reference scale-based social assessments.

Deployment of the developed methodology can repeatably and transparently assess international value chains, highlighting likely impact hotspots. The result is more efficient resource use concerning impact-related due diligence. Significant value can be seen within the setting of industrial strategic decision-making, expanding the understating of social risk, and accelerating mitigation efforts.

As an example of utility in decision-making support, a process relying on large process water feed rates (e.g. metal surface finishing) would be more sensitive to deployment in regions exhibiting poor performance within the 'risk of change in access to water' indicator. With this identified as a potential issue at an early stage, additional precautions can be taken to ensure that the process is relocated, or that water demands are not met at the detriment of societal stakeholders.

As identified in the literature and earlier sections of this paper, the complexity of social impact pathways represents a significant and recognised challenge. An ideal scenario would incorporate hyper-granular data, detailing every included community, allowing for the accurate tracing of impact propagations. In this, temporally accurate, bespoke models would be required for every constituent community, accurately reflecting cultures, local behaviours, attitudes, and needs. This is a significant and potentially impossible task. Consequently, this paper's proposal of red-flag-based value chain assessments provides a pragmatic and balanced solution. With risk hotspots identified, available energy and resources can be accurately deployed to formulate bespoke mitigation strategies.

Indicator selection is far from uniform within the SIAs observed in the literature, an unavoidable consequence of highly diverse goal and scope requirements. However, it is recommended that impact pathway-oriented SIA CMs continue to be developed in a manner aligned with the impact categories and sub-categories found within the UNEP and SETAC guidelines. These are selected due to their wide acceptance as the gold standard within SIA practitioner guidance. Furthermore, the development of competing CMs, as seen in LCA, often further fragments the field. If commonality can be achieved in the CMs used by practitioners, more meaningful inter-assessment comparisons can be made, adding significant value to all stakeholders.

A final notable step taken in this work is the delivery of fully quantified impact indicator results, replacing the semi-quantitative values produced via reference scales. In this, a greater degree of granularity is realised through the use of a continuous scoring scale. Differences between competing alternatives can, therefore, be examined in higher resolution, avoiding the (typically) five-point scales seen in existing work.

While significant future work is required to reach the maturity seen in LCA CMs, the concept can be viewed as proven, albeit on a modest scale.

6 Proof-of-Concept Study

6.1 Introduction

As the final major chapter of this thesis, the work herein covers the application of the previously developed hub and spoke framework and SIA characterisation models to a relevant FMCG use case. Soda Ash production for use within Unilever Home Care products is adopted as the subject of an initial study. While soda ash oriented assessments are present in literature, as revealed through a later review, they are typically very limited in scope and exhibit concerning degrees of opacity with respect to their employed LCI data; a characteristic that is hopefully remedied via this work. The approach taken in this study, the assessed product, and the value chain character will now be introduced sequentially.

6.1.1 A Proof-of-Concept

Within this chapter, these novel methodologies will be employed simultaneously to deliver a proof-of-concept assessment that evaluates their effectiveness. Given the FMCG and CDU focus of the two methodologies, the product system assessed within the proof-of-concept study must reflect these research areas. As noted in Chapter 5, the geographic location of pre-deployment CDU (and FMCG) value chains is often only loosely defined (usually considered at the national level). This is indeed true within this Unilever instigated study. As part of the 'Clean Future' initiative [16], Unilever Home Care have commissioned a screening assessment of Asia-Pacific (APAC) Soda Ash production, focussing on production and usage in India. As a consequence of this geographic focus, the hub process examined will be modelled to reflect an Indian locale. However, an average deployment case will be evaluated, avoiding the selection of a final plant location that nominally occurs later in the value-chain's development.

Despite targeting insight generation around the APAC production of soda ash, the primary aim of this proof-of-concept is to evaluate the efficacy of the developed assessment framework and SIA characterisation models. Simultaneously, their performance will be examined for potential shortcomings and opportunities for future development. A range of primary, or hub, processes are examined for their CDU applicability, representing purple carbon usage within Unilever's 'Clean Future' initiative (see Figure 1-3). Once identified, the best suitor is carried through into a full hub and spoke holistic assessment (cradle-to-gate scope). Consequently, multiple feedstock options must be examined for each process input, primarily focussing on Indian and Chinese production locations (owing to China's manufacturing capacity and market proximity). A broad suite of indicators, spanning the three assessment strands, are selected on a semi-systematic basis. LCIs / LCIAs for the hubs and spokes are subsequently produced, their impacts quantified, and all possible value chain permutations assessed.

Once complete, the assessment results are dissected to reveal any additional insight generation from the framework's application that supports industrial or FMCG decision making. This includes the determination of the value chains' objective impact indicator results on the basis of one tonne of soda ash produced. In addition, the certainty with which the framework can recommend value-chain components or suppliers, and the influence of decision maker MCDM value choices on the selection of the most appropriate value chain alternative, are evaluated.

6.1.2 Soda Ash Manufacturing

For thousands of years soda ash (Na_2CO_3) has been a critical feedstock in processes that make modern societies recognisable. It is well evidenced that ancient Egyptians mined dried lakebed deposits on large scales to obtain natural soda ash; this was subsequently used to produce glass ornaments and jewellery. In modern times it can be found from large scale glass making and metallurgy, to powered detergents (as is the case for Unilever Home Care) and cosmetics. It is of such importance that the Federal Reserve Board uses soda ash production data as a factor in determining indicators that monitor the condition and health of the U.S. economy.

Worldwide, 16,200,000 tonnes of soda ash were exported in 2018 [239]. The total market size, inclusive of domestic usage and sales, was estimated at 57,500,000 tonnes in 2019 [240]. Globally, the soda ash market was in growth throughout the first half of the 2020's, increasing to 65,940,000 tonnes by the end of 2024 [241]. Of this, around 1,500,000 tonnes of soda ash are sold annually by fast moving consumer goods (FMCG) company Unilever as a constituent of powdered washing detergents, contributing roughly a third of the formulation by weight [242]. Its incorporation improves cleaning properties and product efficiency via its abilities to; act as a builder to emulsify oil and alcohol-based soiling, increase alkalinity for pH adjustment, soften the washing liquor (Ca^{2+} and Mg^{2+} removal), and action as a surfactant carrier. These powdered detergents are primarily sold in developing markets such as India, and Indonesia. Consequently, it is expected that use within the APAC region will experience a CAGR of 5.3% until 2030 [243], significantly bolstering base soda ash demand. Furthermore, reports show that powder-based products make up the largest segment within the global detergent market, accounting for 31% of total revenue in 2016 [243]. Market research carried out by Unilever in India showed that 93% of laundry is done using soda ash based powdered detergent [242]. This use in soaps and detergent sconstitutes a significant ~15.8% share of global soda ash production [244]. With industrial usage at these magnitudes, significant environmental, economic, and social benefits can be realised by even small incremental improvements in the utilised value chain(s).

Currently, China and the United States are the primary producers of soda ash, with Russia, Turkey, Germany, and India having established themselves as notable secondary production markets (Figure 6-1). However, production shares are likely to remain highly dynamic due to both on-going and proposed capacity expansions. For instance, Turkey has seen two recent investments in capacity; a 500,000-tonne upgrade at the Ciner Group's Beypazari plant, and the start-up of a new 2,500,000 tonne facility at Kazan [239]. Both of these capacity expansion projects produce soda ash from trona for export. Trona, in contrast to synthetic routes, is an easily refinable, natural resource, rich in sodium carbonate (soda ash). US producers are also proposing additional capacity; with Solvay targeting a 600,000-tonne expansion, 1,000,000 tonnes from Ciner Group, as well as a 680,000-tonne upgrade from Genesis Alkali [245]. These upgrades to existing facilities are expected to be augmented further by the start-up of two new Ciner Group plants, each with a 2,500,000-tonne capacity, around 2025 [245]. Although, these projected timelines may be extended due to suspensions caused by the uncertainty, and other legacy impacts, associated with COVID-19 on international markets.

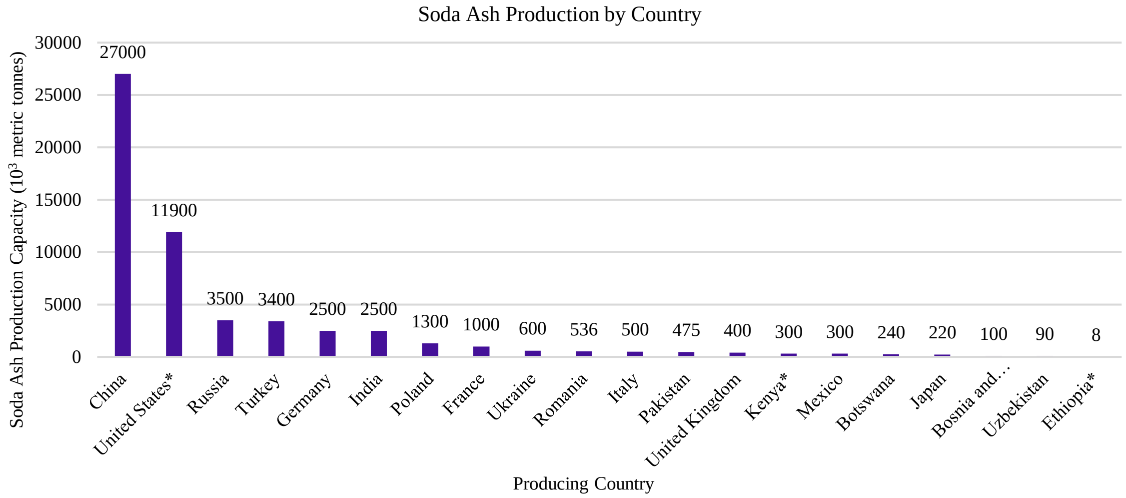


*Figure 6-1 - Annual soda ash production in 2019 by country. Data obtained from U.S. government reporting [246], excluding minor producers with uncertain data. *Only natural production via trona mining.*

With generally highly optimised processes, an average CO_2 emission rate of 1,135kg per tonne of soda ash is realised by industrial Solvay based producers [247]. With this emission rate and the current production volumes, soda ash value chains appreciably contribute to global warming (approx. 79,842,000 tCO_2 p.a.). However, the presence of a carbonate group (CO_3^{2-}) within the product offers potential for the deployment of carbon dioxide utilisation (CDU). Through this, cradle-to-gate net CO_2 emissions may be reduced. The difficulty lies in a classical CDU issue; CO_2's inherent thermodynamic stability. This brings with it significant transformation or valorisation-based energy requirements, likely exceeding those of more traditional and established production routes. If an economically and socially feasible net zero soda ash value chain could be identified and rolled out, both global and local communities, as well as industry, would benefit; manifested through the avoidance of potential future carbon tariffs, and enhanced environmental stewardship. In order for this opportunity to be realised, existing routes must first be examined for their fitness to incorporate CDU. With new facilities planned, such existing routes and processes will persist and operate at scale for multiple decades. Any improvements will therefore have a valuable and significant cumulative effect. Low technology readiness level (TRL) processes will not be considered due to their lesser throughputs and lack of suitability for immediate utilisation in FMCG value chains. In essence, while the development of low TRL or novel processes is a key aspect of the transition towards sustainable industry, those currently at industrial scale use must also be examined to identify options for immediate improvement. Furthermore, low TRL processes are difficult to assess comparatively due to discrepancies in their development phases and optimisation efforts [19].

6.2 Aims, Objectives & Narrative Structure

The main aim of this chapter is to exercise the developed assessment framework and social impact characterisation models. Developed in abstraction, the benefits they deliver cannot be known with certainty without a representative application. Consequently, a proof-of-concept acts as a conclusive evaluation of their efficacy and value addition. A business relevant CDU and FMCG oriented application has been identified in APAC soda ash production. While aiming to deliver insights into the performance of soda ash value chains, time constraints require that the LCI data set be generated and evaluated on a screening basis. Consequently, aspects such as transportation and the sensitivity analysis have been omitted. While it must be recognised that this fact detracts from the certainty and resolution of the generated impact indicator results, the evaluation of the methodologies is unaffected. Furthermore, at early investigative stage stages of value chain development, the exact transportation distances or modes are unlikely to be known, minimising the consequence of their exclusion.

Table 6-1 – Research objectives for the proof-of-concept study

Objective	Specification
4.1	Identify and characterise the major incumbent soda ash production routes.
4.2	Evaluate the major synthetic soda ash production processes for CDU potential and select the most promising for a full assessment.
4.3	Generate a set of demonstration hub and spoke LCIs based on the selected soda ash production process to verify the efficacy of the standardised data sheet developed in Chapter 4.
4.4	Demonstrate the conduction of a holistic sustainability assessment using the developed framework around the selected soda ash production process.
4.5	Evaluate the effectiveness of the model's value chain selection approach and rank reversal induced by decision maker value choices.

In a departure from the relatively uniform and formulaic narratives seen in the preceding three chapters, the work herein adopts a less linear form. Given the overarching purpose of this chapter, the application and evaluation of the methodologies developed in Chapters 4 and 5 within a FMCG relevant case-study, call backs and sub-case studies are utilised. These are focussed within section 6.6 and detailed visually in Figure 6-2. The most prominent example is a pause to demonstrate the procedure used to generate LCIs for the assessment's spoke processes (Section 6.6.3). Given the total spoke count of 35 within this proof-of-concept assessment, it was deemed infeasible to independently chronicle the collection and handling of their constituent data. Instead, this sub-case study examines the environmental LCI and LCIA phases of the grid mix spokes, the process for which is representative of all other spoke sets deployed within the proof-of-concept.

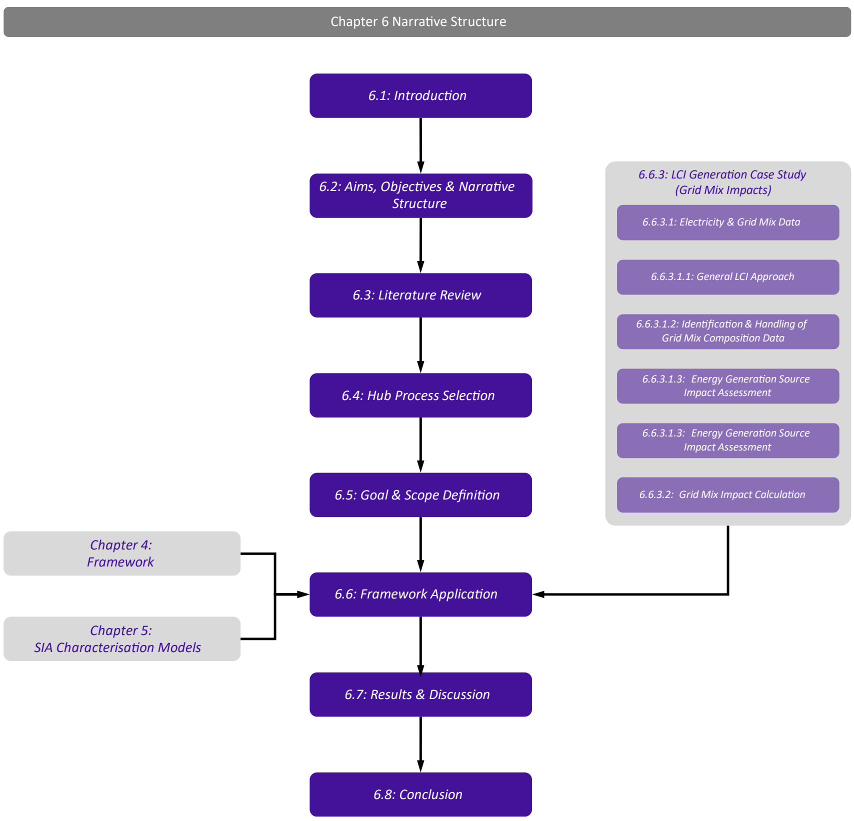


Figure 6-2 – Narrative structure of chapter 6.

6.3 Literature Review

This review initially focusses on the identification and characterisation of large-scale soda ash production routes relative to a global context. Within this, each of the identified processes is outlined before their constituent reaction steps are evaluated. Following this, pertinent existing assessments are collated, with their results being examined in terms of magnitude as well as quality and transparency. Finally, any attempts at CDU integration to soda ash production, or lack thereof, are extracted from literature and evaluated.

6.3.1 Major Production Routes

Soda ash can be sourced either naturally or synthetically. As shown by Figure 6-3, the Solvay process supplies a significant majority of the synthetic market, representing 48% of total global production in 2014 (more recent differentiated route data was not available in open literature at the time of writing). Alternative synthetic routes are also utilised, generating another 25% of annual production, with the remaining 27% procured via natural sources [248]. The 25% of global synthetic production attributed to non-Solvay routes is dominated by the Hou process, primarily deployed in China, being minorly supplemented by the modified Solvay process [249].

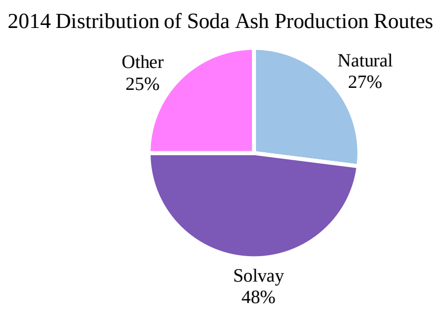


Figure 6-3 - Breakdown of soda ash production capacity by route, based on literature data [248].

6.3.1.1 Solvay Process

Developed in 1861, the Solvay process produces high purity soda ash using sodium brine and limestone. An ammonia saturated sodium brine solution is contacted with CO_2, obtained from the pyrolysis of lime. This results in the generation of sodium bicarbonate and ammonium chloride. Ammonia, while not present in the overall reaction, plays an important role in the buffering of the solution within the Solvay tower at a basic pH. Without this action the precipitation of sodium bicarbonate ($NaHCO_3$), from which soda ash is obtained, will be prevented [250]. Calcium oxide from the lime pyrolysis is hydrated to generate slaked lime for ammonia recovery. It quickly became the dominant method for synthetic soda ash production owing to its closed-loop nature that minimises waste and pollution relative to earlier soda ash production methods such as the Le Blanc process [251] [252]. Despite this, the Solvay process still generates significant CO_2 emissions, potentially reaching 1.9-tonnes of CO_2 per tonne of soda ash [253]. Alone, the use of calcium oxide derived from pyrolyzed lime results in a minimum step specific net CO_2 emission of one mole per mole of soda ash [254]. Consequently, the process is stoichiometrically prevented from reaching a carbon negative status.

Table 6-2 - Shows reactions occurring within the Solvay Process [255] [256]

Reaction	Corresponding Step
$CaCO_3 \rightarrow CaO + CO_2 \uparrow$	1
$2NH_3 + 2CO_2 + 2H_2O \leftrightharpoons 2NH_4HCO_3$	2
$2NH_4HCO_3 + 2NaCl \rightarrow 2NaHCO_3 \downarrow + 2NH_4Cl$	3
$2NaHCO_3 \rightarrow Na_2CO_3 + CO_2 \uparrow + H_2O$	4
$CaO + H_2O \rightarrow Ca(OH)_2$	5
$2NH_4Cl + Ca(OH)_2 \rightarrow 2NH_3 \uparrow + CaCl_2 + 2H_2O$	6
$2NaCl + CaCO_3 \rightarrow Na_2CO_3 + CaCl_2$	*OVERALL*

6.3.1.2 Modified Solvay Process

Process iteration led to the modified Solvay process, removing the requirement for NH_3 within the original process and therefore the energy associated with its recovery. Furthermore, it delivers the capability to use captured CO_2 as a feedstock. Calcium oxide is added directly to the column, contacting the brine, and producing calcium hydroxide for the reaction. This increases the pH, negating the need for NH_3 as seen in the original process [257]. While this offers potential benefits in terms of net CO_2 emissions, the sourcing of calcium oxide from routes other than limestone pyrolysis may prove problematic at large scales. An alternative to the calcium oxide feed is to supply the process directly with a calcium hydroxide feedstock; a significant by-product of acetylene production, formed at a rate of 2.8t calcium hydroxide per tonne acetylene [258]. This would reduce industrial waste and facilitate the downstream utilisation of captured CO_2. Despite these potential advantages, the formation step of $NaHCO_3$ is more exothermic than its traditional Solvay equivalent, resulting in elevated cooling duties, representing a potential detractor.

Table 6-3 - Reactions occurring within the modified Solvay process [257]

Reaction	Corresponding Step
$CaO + H_2O \rightarrow Ca(OH)_2$	1
$2NaCl + 2CO_2 + Ca(OH)_2 \rightarrow CaCl_2 + 2NaHCO_3 \downarrow$	2
$2NaHCO_3 \rightarrow Na_2CO_3 + CO_2 \uparrow + H_2O$	3
$2NaCl + CO_2 + Ca(OH)_2 \rightarrow Na_2CO_3 + CaCl_2 + H_2O$	*OVERALL*

6.3.1.3 Hou Process

The first few steps of the Hou process are comparable to these of the Solvay process; ammonia and carbon dioxide are dissolved in aqueous sodium chloride to produce sparingly soluble sodium bicarbonate, which is calcined to sodium carbonate [259]. However, where the Solvay process recovers the ammonia in a recycle loop, the Hou process does not. It is notable that the Hou process does not require a calcium source like both iterations of the Solvay process. Consequently, calcium chloride is not produced as a waste stream, instead ammonium chloride is formed. This can be refined through additional steps to form fertiliser as a co-product [260]. Ammonium chloride and soda ash are produced in almost equal quantities; two moles (107 g) of ammonium chloride are produced for each mole (106 g) of soda ash. The route is less widely used than the Solvay process, being deployed primarily in China. However, crucially for the scope of this work, the use of CO_2 as a feedstock theoretically permits the attainment of carbon negative soda ash.

Table 6-4 - Reaction scheme within the Hou Process

Reaction	Corresponding Step
$2NH_3 + H_2O + CO_2 \leftrightharpoons (NH_4)_2CO_3$	1
$(NH_4)_2CO_3 + CO_2 + H_2O \leftrightharpoons 2NH_4HCO_3$	2
$2NH_4HCO_3 + 2NaCl \leftrightharpoons 2NaHCO_3 + 2NH_4Cl$	3
$2NaHCO_3 \rightarrow Na_2CO_3 + H_2O + CO_2$	4
$2NaCl + 2NH_3 + CO_2 + H_2O \rightarrow 2NH_4Cl + Na_2CO_3$	*OVERALL*

6.3.1.4 Natural Soda Ash (Trona Mining)

A majority of natural soda ash is extracted from trona ore or sodium carbonate rich brine, found in ~95 sites globally [261]. These resource deposits are vast, with Green River Basin in Wyoming containing an estimated 47 billion tonnes of extractable soda ash [261], enough to satisfy current global demand (65,940,000 tonnes p.a. [11]) for approximately 800 years. The route involves several steps; ore extraction using underground mining techniques, crushing, calcination, and mixing with water to form a slurry. Finally, this slurry is processed via a series of purification steps and reactions; the exact methods vary based on ore calcination temperature and initial composition [262]. This initial ore is a mixture of primarily; trona (Na_2CO_3•$NaHCO_3$•$2H_2O$), thermonatrite (Na_2CO_3•H_2O) and natron (Na_2CO_3•$10H_2O$). Within these natural deposits, only ores with at least 70.3% Na_2CO_3 content are of commercial interest [262]. Due to the natural origin of this soda ash, there is no scope for CDU. Consequently, it will not be considered further in this work. In addition, the composition of ore can vary, sometimes significantly, with geographical location [262]; this leads to significant difficulty in determining a representative reflection of waste streams and processing steps.

6.3.2 Existing Soda Ash Sustainability Assessments

The route by which soda ash is obtained depends heavily on proximity to natural trona deposits. For this reason, synthetic routes will necessarily persist into the future to meet decentralised demand. Consequently, their optimised performance against environmental, economic, and social indicators is vital. Literature was consulted to identify openly available assessments of soda ash production. LCA was by far the most commonly evaluated strand, resulting in the publications collated within Table 6-5. The GWP values presented by these publications, along with their studied process and comments on the assessment are also presented. TEA and SIA studies are discussed latterly, a consequence of their low publication count.

Table 6-5 - Existing LCA's for the production of soda ash via major routes

Existing Soda Ash LCA's					
Net CO_2 eq. per ton SA	Process	Location	Notes	Reference	Year
1.85	Solvay	Not Specified	No information regarding how data was acquired or generated	[263]	2015
1.4	Natural	USA	Can't see background data	[253]	2015
1.9	Solvay	USA	Can't see background data	[253]	2015
2.2	Hou	USA	Can't see background data	[253]	2015
0.5	Trona	USA	Can't see background data	[264]	2015
0.7	Trona	USA	Can't see background data	[264]	2015
0.9	Solvay	EU	Can't see background data	[264]	2015
1	Hou	China	Can't see background data	[264]	2015
0.75 (only CO_2)	Trona	Not Specified	Only a value for 'CO_2 emissions factor' presented, not CO_2-Eq..	[265]	2019
1.05 (only CO_2)	Hou	Not Specified	Only a value for 'CO_2 emissions factor' presented, not CO_2-Eq..	[265]	2019
1.10 (only CO_2)	Solvay	Not Specified	Only a value for 'CO_2 emissions factor' presented, not CO_2-Eq..	[265]	2019
1.35 (only CO_2)	Solvay	Europe	Only a value for 'CO_2 emissions factor' presented, not CO_2-Eq..	[266]	2017

While multiple LCA sources in open literature give a figure for the GWP associated with soda ash production, a vast majority are not transparent or reliable in nature. With none disclosing their underpinning LCI data, or the methodology and characterisation models employed, it is impossible to verify, validate, or reproduce the findings. What can be said with confidence is that beyond GHG emissions, the impact indicators selected are both sparse, and far from uniform across the identified assessments. The range of indicators evaluated within the assessments is detailed by Table 6-6.

Table 6-6 - Impact indicators evaluated within previous soda ash assessments.

Reference / Source	Impact Indicators								
	CO_2 (or CO_2-Eq)	Eutrophication Potential	Acidification Potential	Ozone Depletion	Photochemical Ozone (Smog)	Respiratory Health	Mineral Resource Depletion	Human Toxicity	Aquatic Toxicity
[263]	✓	✓	✓	✓	✓	✓	✓	✓	✓
[253]	✓		✓	✓	✓				
[264]	✓								
[265]	✓								
[266]	✓								

Carried out independently by Sustainable Solutions Corporation, the Industrial Minerals Association report is the most compelling of those identified; purportedly ISO 14040 compliant and peer reviewed, it assesses three of the major routes examined in Section 6.3.1 [253]. However, the study does not give any supporting information such as the sources of feedstocks and energy. Critically, it also omits LCI data, preventing any detailed analysis, validation, or replication.

Prashantsinh, *et al*. use LCA software (Gabi) to complete a cradle-to-gate assessment for the Solvay process. Again, no data, assumptions or methodology are disclosed, reporting only impact indicator values. However, interestingly, the results show that ~89% of GHG emission can be attributed to the carbonation and ammonia recovery steps [263], suggesting CO_2 lost from the carbonation tower is not recycled in this specific system.

A sectoral case study of soda ash, conducted by the Centre for European Policy Studies (CEPS) [264] focusses on existing coal and gas fired plants. These values are therefore not of significant interest under Unilever's Clean Future' initiative due to reliance on fossil carbon. The lowest GHG emissions figures found were those of Solvay, claiming 1.05-1.10 tCO_2/t SA for synthetic routes and 0.45-0.75 tCO_2/t SA for natural routes [265]. These figures are internal estimates within the company and its partners, with no data reenforcing the emissions levels provided.

In 2017 the EU's JRC science for policy report provided the most transparent LCA of soda ash found in open literature. It provides tables of typical process inputs per tonne of soda ash, both material and energy, followed by descriptions of, and comments on, the unit operations, conditions, and assumptions made. Multiple plants have been considered in the assessment, with emissions ranging from 0.7-2.0 tCO_2/t SA [266]. The average of these two values is used to give the estimated average emissions of soda ash production as 1.35 tCO_2/t SA. However, this figure does not include the production or transportation of feedstocks. Consequently, underestimating the emissions when compared to a cradle-to-gate assessment. The thermal energy is also obtained from burning either natural gas or coal, a non-ideal scenario under Unilever's 'Clean Future' initiative. Both sources represent a deviation from the objectives of this project. A significant limitation is also found in the consideration of only one impact indicator.

Economic and social impact assessments around soda ash production are relatively sparse, assumedly due to commercial sensitivity. The identified technoeconomic assessments instead focus on the scrubbing of CO_2 from the Solvay process for conversion to other value-added chemicals such as methanol [267]. However, they give the estimated total cost of production (TCP) for soda ash production with and without CDU, 305.4 and 156.3 €/t respectively. This assessment will prove useful for insight as CO_2 capture will be employed in some supply chains examined.

One SIA is present in literature covering the production of soda ash [268]; however, it is methodologically outdated (published in 2007, thus predating the UNEP and SETAC guidelines) and takes approaches in which the exact geographical location must be known. This requirement for a specified deployment location makes the implementation and use of the framework a significant challenge (e.g. calculating loss of housing). It is instead more applicable to employ the UNEP/SETAC guidelines [269] or triple helix framework [7] inspired characterisation models derived in Chapter 5.

Generally, this section of the literature has revealed a significant lack of open-source knowledge around the sustainability assessment of soda ash production. Considering its significance in modern society, this is initially a surprising result. However, when considering the value of the global soda ash market (20.89 billion USD in 2022 [270]) perhaps it should be expected. Commercial sensitivity around the processes' operation and performance optimisation results in LCAs and TEAs that are of significant value to producers, offering competitors an insight into any potential or perceived competitive advantages. The lack of SIA studies is less attributable to this, particularly in the case of reference scale based assessment that do not usually contain primary process data. Instead, the absence of publication in the area are attributed to the youth of the assessment strand and it's perceived lesser value to corporate organisations.

6.3.3 CDU Application Within Soda Ash Production

Following a second round of literature searching, very few studies are identified around the integration of CDU within the synthetic soda ash production routes. Web of Science was again used to collect relevant publications using the keyword search terms;

- Soda ash, and;
- CDU, or;
- CCU, or;
- CCUS, or;
- Carbon Dioxide Utilization, or;
- Carbon Dioxide Utilisation, or;
- Carbon Capture Utilisation and Storage, or;
- Carbon Capture Utilization and storage

Through this approach only a handful of useful publications were returned, each offering various degrees of relevance; a suspected consequence of soda ash production's recognition as a 'hard to abate sector' in terms of CO_2 emissions [271].

Collated studies, along with their focus and relevant notes are given in Table 6-7. The literature that is present reveals an almost sole focus on the Solvay process as a vehicle for CDU deployment with respect to soda ash production. The modified Solvay process is identified and considered within one publication from Quang *et al.*

[254], with the Hou process ignored entirely. While this can be partially attributed to the dominance of the Solvay process in the production of synthetic soda ash (as shown in Figure 6-3), the consequential neglect of the modified Solvay and Hou processes in these considerations may result in overlooked CDU opportunities; and, in turn, cleaner soda ash.

Examining the identified literature around CDU and the Solvay process, several key themes are observed. Quang *et al*. recognise the general importance of CDU adoption by the soda ash industry if emissions are to be reduced, stating that none of the CDU approaches currently identified are nearing industrial deployment and suggesting that CDU is currently focussed on the utilisation of CO_2 within waste stream management [254]. This conclusion is reenforced in the works by Rumayor *et al*. [271], Czaplicka and Konopacka-Łyskawa [272], and Cao *et al*. [273] noted in Table 6-7. The utilisation of liquid waste is one of the most pertinent issues in the area. Disposal of these streams directly to surface waters often results in strong salinity within nearby groundwater, natural reservoirs, and soil [274].

Table 6-7 - Literature identified through Web of Science covering soda ash related CDU deployment.

Publication	CDU Focus	Comments	Reference
The Utilization of CO_2, Alkaline Solid Waste, and Desalination Reject Brine in Soda Ash Production	Review of the adaptations proposed to integrate CDU within the Solvay process.	No high TRL technologies recommended.	[254]
CO2 utilization from power plant: A comparative techno-economic assessment of soda ash production and scrubbing by monoethanolamine	Comparison of a novel NaOH soda ash route for NGCC relative to existing flue gas scrubbing.	Novel process that does not utilise or benefit currently deployed processes. Consequently, this publication is outside of this paper's scope.	[275]
Toward the Decarbonization of Hard-To-Abate Sectors: A Case Study of the Soda Ash Production	Examines the potential coupling of soda ash production with other CDU technologies to utilise CO_2 from the traditional Solvay process.	Focussed more on CDU oriented methanol production with the Solvay process as a CO_2 source for a technoeconomic assessment case-study. Technoeconomic assessment did not indicate current viability unless factors such as wholesale renewable electricity or CO_2 process shift in favour of CDU deployment.	[271]
Studies on the utilization of post-distillation liquid from Solvay process to carbon dioxide capture and storage	Adaptation of the Solvay process to utilise waste distillation sludge for CO_2 mineralisation to form calcium carbonate.	Product produced is of economic value. While not incorporating captured CO_2 into the product itself a direct by-product is generated. Technoeconomic assessment indicated that the route modification is viable.	[272]
Technoeconomic Analysis of a Brine Purification Process - Combined Carbon Dioxide Mineralization and Hydromagnesite Recovery	Adaptation of the Solvay process to utilise a waste stream for CO_2 mineralisation.	Both waste management and CO_2 mineralisation are achieved simultaneously through the mineralisation of CO_2 within the Solvay process' brine purification sludge. Calcite and Hydromagnesite are generated. Technoeconomic assessment suggested that the route modification is viable.	[273]

Both the brine purification and distillation sludges contain alkali metals which can be mineralised into their respective carbonates. If of suitable quality, these CDU opportunities may also result in additional saleable products, for example, use as a cement aggregate; also serving to further reduce CO_2 emissions by substitution. The relatively low TRL state of waste management techniques within soda ash production is a persisting issue, extending beyond the confines of CDU approaches [276] [277] [278] [279]. This fact supports pressure for a multi-pronged approach to industrial sustainability; on one hand developing cleaner and novel primary processes, while on the other optimising the impacts of existing value chains to support the interim transition period prior to industrial scale roll out of the novel routes. The lack of literature around CDU potential in the modified Solvay and Hou processes represents a clear gap in knowledge.

This chapter's proof-of-concept study aims to validate the developed methodologies and therefore will focus on a single hub process, and it's associated spoke sets. However, in recognition of Unilever's 'Clean Future' initiative, the study's orientation around the process with greatest CO_2 uptake potential is desired. This will facilitate the evaluation of purple carbon (see Figure 1-3) as a process feedstock, and its consequential effects on the value-chain's impact profile. Ideally, the full hub and spoke assessment would be carried out for each of the three core production processes. However, in recognition of this project's constraints, this must be limited to a single assessment. To inform the selection of a process for deeper analysis, a systematic screening assessment of CO_2 uptake potential across the full suite of current deployed processes and routes (Solvay, modified Solvay, and Hou) must be conducted, benefiting the effectiveness of future value chain selection and identification.

6.4 Hub Process Selection

This section examines the applicability of CDU within the three dominant synthetic soda ash production routes. Quantification is achieved through the examination of process chemistry and the constituent reaction steps. Through this approach, coarse but useful insights are generated around the best available CDU opportunity. A theoretical CO_2 uptake is calculated for each process relative to a functional unit of 1 tonne of soda ash. However, in the pursuit of low net emissions, CDU will only be considered viable when uptake outstrips the process' direct CO_2 emissions. For example, a process with a maximum theoretical CO_2 uptake of 0.4 kg/kg_{prod} with direct emissions of 0.3 kg/kg_{prod} will yield a maximum CDU potential of 0.1 kg/kg_{prod}. The economic and social assessment strands, as well as additional LCA indicators, are not considered in this initial screening as they do not directly influence the CDU capability of the system.

The handling of wastes and production of feedstocks excluded from the assessment due to the full proof-of-concept assessment's cradle-to-gate scope; consequently, consideration at this stage would hinder progress while providing no additional utility. Electricity is excluded due to significant geographic sensitivity; for instance, the renewable portion of grid mixes ranges from 0 (Bahrain, Oman, etc.) to 0.9624 (Congo) [280]. The result of this screening study system boundary is the sole consideration of the direct stochiometric emissions associated with the soda ash production processes. These represent the only aspect of its production that is unalterable without the deployment of fundamentally novel routes and technologies. Consequently, a fair comparison is reached between routes.

6.4.1 Process Outline & BFDs

Primitive process models are developed to quantify the direct emissions of the Solvay, Modified Solvay, and Hou processes respectively. These are built around the reaction steps defined in Table 6-2, Table 6-3, and Table 6-4. Block flow diagrams (BFDs) including the major process units are constructed and recycle loops integrated. In the interest of comparability, filters, condensers, and mixers are assumed to be 100% efficient; while this adds uncertainty, it is deemed reasonable for such an initial screening study. These BFDs and assumptions are used to complete stream tables for the production basis of 1 tonne soda ash. Excel is chosen for this task to facilitate sensitivity analysis, examining the effect of each reaction step's conversion efficiency on the net stoichiometric CO_2 uptake or emission. Scenarios are then assessed to identify the best possible performance of each option and quantify CO_2 emissions per tonne of soda ash produced.

The BFDs for the process are given by Figure 6-4, Figure 6-5, and Figure 6-6. Due to the choice to exclude the waste stream, feedstock, and energy related emissions, ancillary units such as heat exchanger, compressors and pumps are excluded. The exception to this rule is condensers, where the unit inclusion is necessary to model the splitting of stream components. Green and red streams represent incoming and outgoing boundary flows respectively.

6.4.1.1 Solvay Process

The Solvay process (detailed by Figure 6-4) is the most complex of the three examined routes in terms of both unit count and reaction steps. This can be largely attributed to the recovery of the ammonia, adding two additional major units (ammonia recovery tower and absorber). This closed ammonia loop is given by streams, 12, 11, 9, 14, and 13 in sequence. Stream 3 represents ammonia top-up in the event that the recovery cycle (reaction steps 5 and 6 in Table 6-2) introduces minor losses as NH_4Cl in stream 17. CO_2 is not fed to the stream directly, rather it is obtained through the pyrolysis of lime in reaction step 1 (first seen in stream 4). Steps 2 and 3 take place in the Solvay tower, precipitating sodium bicarbonate for subsequent separation (stream 8). Once separated, reaction step 4 occurs with the addition of heat in the calcinator, generating soda ash, water vapour and CO_2. The CaO produced with CO_2 in reaction step 1 is slaked during step 5 and finally used to recover ammonia from the aqueous NH_4Cl within stream 9 during step 6.

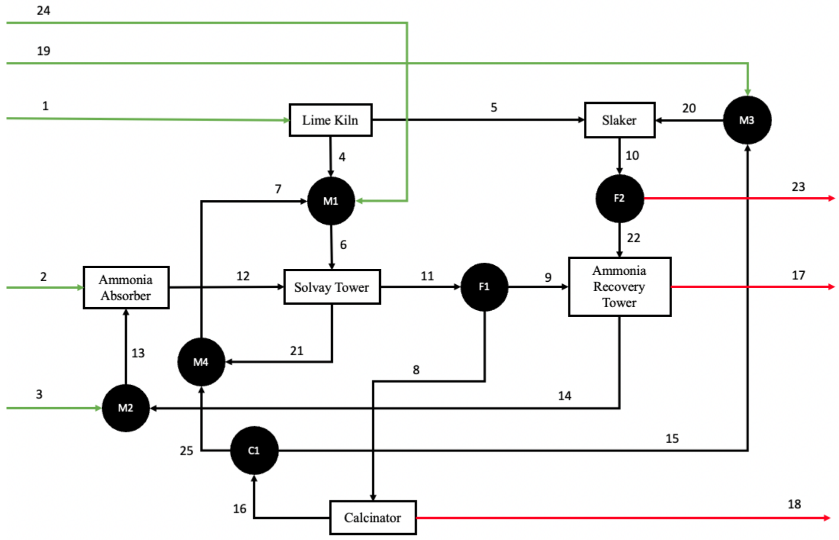


Figure 6-4 - BFD for the Solvay Process

6.4.1.2 Modified Solvay Process

Figure 6-5 shows the modified Solvay process. The primary difference being the omission of the lime pyrolysis step. The lack of ammonia recovery is also notable, with a 50% reduction in terms of both reaction steps and major process units. Unreacted CO_2 is recycled for a second pass from the bubble column gas outlet (stream 6) after mixing with additional CO_2 from the calcination of the precipitated $NaHCO_3$, represented by stream 12. If additional captured CO_2 is required, this is supplied via stream 8. Reaction step one, slaking of CaO, is dependent on the selection of CaO or $Ca(OH)_2$ as the calcium source. Step 2 occurs in the bubble column, resulting in the formation and precipitation of $NaHCO_3$. Step 3 is the calcination of $NaHCO_3$, as also seen in the traditional Solvay process. Filter 1 (F1) is included to prevent the advancement of unreacted CaO through the process. It should be noted that the identification of CaO or $Ca(OH)_2$ sources on the required scale is a challenge, often this results in reversion to the traditional Solvay process and the associated calcination of limestone.

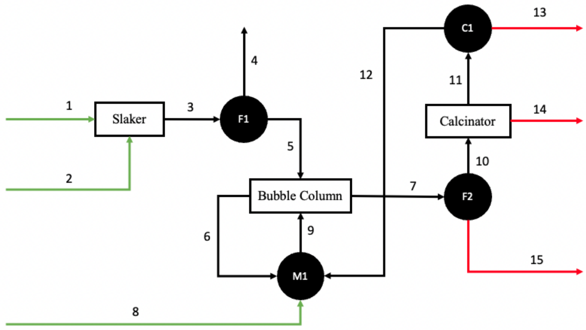


Figure 6-5 - BFD for the Modified Solvay process

6.4.1.3 Hou Process

The final route examined, the Hou process resides between the Solvay and modified Solvay processes with respect to complexity. The process BFD (Figure 6-6) details four major process units, with the same number of reaction steps. A major difference presents itself in the generation of two products, soda ash (stream 15) and ammonium chloride (stream 13). Unreacted CO_2 is again assumed to be recycled and mixed with the calcination off-gas via streams 4 and 5. In the event that stoichiometrically released CO_2 falls short of requirement, stream 6 supplies captured CO_2.

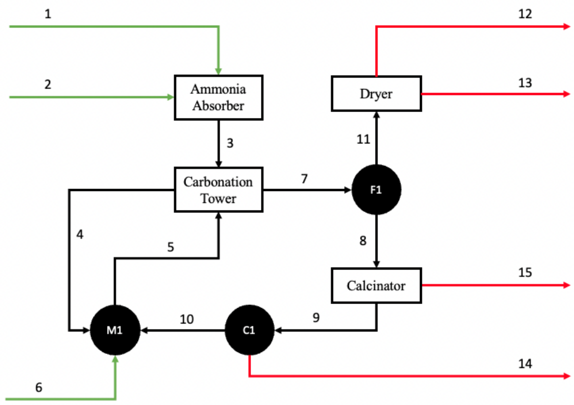


Figure 6-6 - BFD for the Hou process

6.4.2 Process Stream Tables

Using the BFDs stream tables are generated. Mole balances are carried out via Initial, Change, Equilibrium (ICE) tables over units containing reaction steps. Molar flow rates are also converted to their mass equivalent for parallel evaluation and ease of interpretation. A basis of 1 tonne of soda ash was continued, the excel model subsequently adjusts input stream flow rates as necessitated by the selected reaction conversion efficiencies. This yields the stream tables seen in Table 6-8, Table 6-9, and Table 6-10 respectively; in their presented form the systems are evaluated based on the assumption of 100% conversion for all reaction steps. These conversion efficiencies are latterly reduced in increments to examine the effect on CO_2 uptake.

Completeness and accuracy are verified through mass balances over both the whole system and each unit in isolation. No notable mass differentials are observed over any individual process units. The input / output mass deviations over the system boundaries are calculated as 0.00146%, 0.00136%, and 0.00043% for the Solvay, Modified Solvay and Hou processes respectively. These differences can be attributed to the accuracy of molecular weights used (4 d.p.). With complete stream tables derived, and reaction step conversion acting as the as independent variables, the sensitivity of CO_2 emission magnitude can be examined quantitatively.

Table 6-8 – Stream table for the Solvay process (assuming 100% conversion at each reaction step).

Stream	Species In (kg/hr)												Totals
	$CaCO_3$	NaCl	NH_3	CaO	CO_2	H_2O	$Ca(OH)_2$	NH_4HCO_3	$NaHCO_3$	NH_4Cl	Na_2CO_3	$CaCl_2$	
1	944.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	944.3
2	0.0	1838.0	0.0	0.0	0.0	566.6	0.0	0.0	0.0	0.0	0.0	0.0	2404.6
3	0.0	0.0	214.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	214.2
4	0.0	0.0	0.0	0.0	415.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	415.2
5	0.0	0.0	0.0	529.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	529.1
6	0.0	0.0	0.0	0.0	1384.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1384.1
7	0.0	0.0	0.0	0.0	415.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	415.2
8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1585.2	0.0	0.0	0.0	1585.2
9	0.0	735.2	0.0	0.0	0.0	0.0	0.0	994.5	0.0	1009.4	0.0	0.0	2739.1
10	0.0	0.0	0.0	0.0	0.0	0.0	699.1	0.0	0.0	0.0	0.0	0.0	699.1
11	0.0	735.2	0.0	0.0	0.0	0.0	0.0	994.5	1585.2	1009.4	0.0	0.0	4324.3
12	0.0	1838.0	535.6	0.0	0.0	566.6	0.0	0.0	0.0	0.0	0.0	0.0	2940.2
13	0.0	0.0	535.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	535.6
14	0.0	0.0	321.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	321.4
15	0.0	0.0	0.0	0.0	0.0	170.0	0.0	0.0	0.0	0.0	0.0	0.0	170.0
16	0.0	0.0	0.0	0.0	415.2	170.0	0.0	0.0	0.0	0.0	0.0	0.0	585.2
17	0.0	735.2	0.0	0.0	0.0	339.9	0.0	994.5	0.0	0.0	0.0	1047.1	3116.8
18	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1000.0	0.0	1000.0
19	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
20	0.0	0.0	0.0	0.0	0.0	170.0	0.0	0.0	0.0	0.0	0.0	0.0	170.0
21	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
22	0.0	0.0	0.0	0.0	0.0	0.0	699.1	0.0	0.0	0.0	0.0	0.0	699.1
23	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
24	0.0	0.0	0.0	0.0	553.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	553.6
25	0.0	0.0	0.0	0.0	415.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	415.2

Table 6-9 – Stream table for the modified Solvay process (assuming 100% conversion at each reaction step).

Stream	Species In (kg/hr)								Totals
	CaO	NaCl	CO_2	$Ca(OH)_2$	H_2O	$NaHCO_3$	$CaCl_2$	Na_2CO_3	
1	529.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	529.1
2	0.0	1102.8	0.0	0.0	170.0	0.0	0.0	0.0	1272.8
3	0.0	1102.8	0.0	699.1	0.0	0.0	0.0	0.0	1801.9
4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	0.0	1102.8	0.0	699.1	0.0	0.0	0.0	0.0	1801.9
6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7	0.0	0.0	0.0	0.0	0.0	1585.2	1047.1	0.0	2632.3
8	0.0	0.0	415.2	0.0	0.0	0.0	0.0	0.0	415.2
9	0.0	0.0	830.4	0.0	0.0	0.0	0.0	0.0	830.4
10	0.0	0.0	0.0	0.0	0.0	1585.2	0.0	0.0	1585.2
11	0.0	0.0	415.2	0.0	170.0	0.0	0.0	0.0	585.2
12	0.0	0.0	415.2	0.0	0.0	0.0	0.0	0.0	415.2
13	0.0	0.0	0.0	0.0	170.0	0.0	0.0	0.0	170.0
14	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1000.0	1000.0
15	0.0	0.0	0.0	0.0	0.0	0.0	1047.1	0.0	1047.1

Table 6-10 – Stream table for the Hou process (assuming 100% conversion at each reaction step).

Stream	Species In (kg/hr)									*Totals*
	H_2O	NH_3	CO_2	$(NH_4)_2CO_3$	NH_4HCO_3	NaCl	$NaHCO_3$	NH_4Cl	Na_2CO_3	
1	339.9	0.0	0.0	0.0	0.0	1102.8	0.0	0.0	0.0	*1442.8*
2	0.0	321.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	*321.4*
3	339.9	321.4	0.0	0.0	0.0	1102.8	0.0	0.0	0.0	1764.1
4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	0.0	0.0	830.4	0.0	0.0	0.0	0.0	0.0	0.0	830.4
6	0.0	0.0	415.2	0.0	0.0	0.0	0.0	0.0	0.0	415.2
7	0.0	0.0	0.0	0.0	0.0	0.0	1585.2	1009.4	0.0	2594.6
8	0.0	0.0	0.0	0.0	0.0	0.0	1585.2	0.0	0.0	1585.2
9	170.0	0.0	415.2	0.0	0.0	0.0	0.0	0.0	0.0	585.2
10	0.0	0.0	415.2	0.0	0.0	0.0	0.0	0.0	0.0	415.2
11	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1009.4	0.0	1009.4
12	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
13	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1009.4	0.0	1009.4
14	170.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	170.0
15	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1000.0	1000.0

6.4.3 Process CDU Potential

Conversion at each reaction step offers a convenient way to assess the impact of process efficiencies on CO_2 emission or uptake rate. Figure 6-7, Figure 6-8, and Figure 6-9, show the processes' net CO_2 flux at varying step specific conversions. Each step is independently evaluated, with 100% conversion assumed for the other steps. A negative y-axis value indicates that the process chemistry is carbon dioxide negative on a stochiometric gate-to-gate basis. The generated curves converge toward optimal performance (100% efficiency at all reaction steps) on the right-hand side of the figures. Through the curves it can be seen that lower efficiencies, in some reaction steps, actually increases the CO_2 uptake potential (e.g. steps 3 and 4 of the Solvay process), an effect observed across all three processes. In contrast to this behaviour, the Solvay process exhibits examples of decreased step conversion efficiency resulting in greater CO_2 emission, the only process to exhibit this character. Generally, the instances where CO_2 uptake is increased by lowered conversion efficiencies are confined to steps directly involved in the generation of soda ash, not those within recycle loops (e.g. reaction step 6 of the Solvay process). However, poor conversion in these steps indicates the loss of carbonate compounds in process waste streams. Furthermore, such process inefficiencies will have detrimental effects on the economic performance of the systems, incentivising the highest possible operating conversion efficiencies. Nonetheless, it is of value to understand whether inefficiencies would result in beneficial or detrimental behaviour with respect to net direct CO_2 emissions. The generally observed character, across all three systems, shows that CO_2 utilisation rates are significantly more sensitive to conversion efficiency at lower values. As the conversion efficiency rises the curves converge rapidly, breaching the ±1kg CO_2 per kg soda ash threshold by 60% conversion efficiency in all cases. This verifies that higher material efficiencies result in a stabilised process performance, with small variations in conditions less likely to cause significant fluctuations in emissions.

The Solvay process' direct CO_2 footprint is clearly heavily dependent on the conversion of steps 3, 4, and 5; as seen by Figure 6-7. Lower conversion efficiency within steps 3 and 4 positively effects the net CO_2 emission, contrasting the degradation in performance seen as step 5 becomes less efficient. Net CO_2 emission results show maximum and minimum extremes of -15.78 tonne CO_2 per tonne soda ash to 7.89 tonne CO_2 per tonne soda ash, occurring at the minimum conversion efficiency of 5% in steps 3 and 5 respectively. By 50% conversion efficiency these values have reduced in magnitude to -0.83 tonne CO_2 per tonne soda ash and 0.415 tonne CO_2 per tonne soda ash respectively; quantifiably confirming the rapid conversion of emission performance.

Lower conversion at reaction step 3 appears to offer notable benefits for CO_2 emissions, exhibiting the highest sensitivity of all steps. However, further examination using the stream table (Table 6-8) reveals that this manifests itself in the elevated generation of undesired ammonium bicarbonate; accounting for reduced conversion to precipitated sodium bicarbonate and ammonium chloride. This, in effect, acts as a carbon sink in the process; while giving beneficial gate-to-gate impacts, it is not known whether the ammonium bicarbonate will degrade post discharge releasing this CO_2 and negating any benefits. Additionally, the loss of the ammonium ions results in elevated feedstock costs and ammonia top-up rates (0.214 tonne ammonia per tonne soda ash at 60% conversion) as recovery will not occur efficiently. This will also bring secondary emission penalties via production of this additional ammonia, potentially emitting up to 3.8 kg CO_2 per kg ammonia [281].

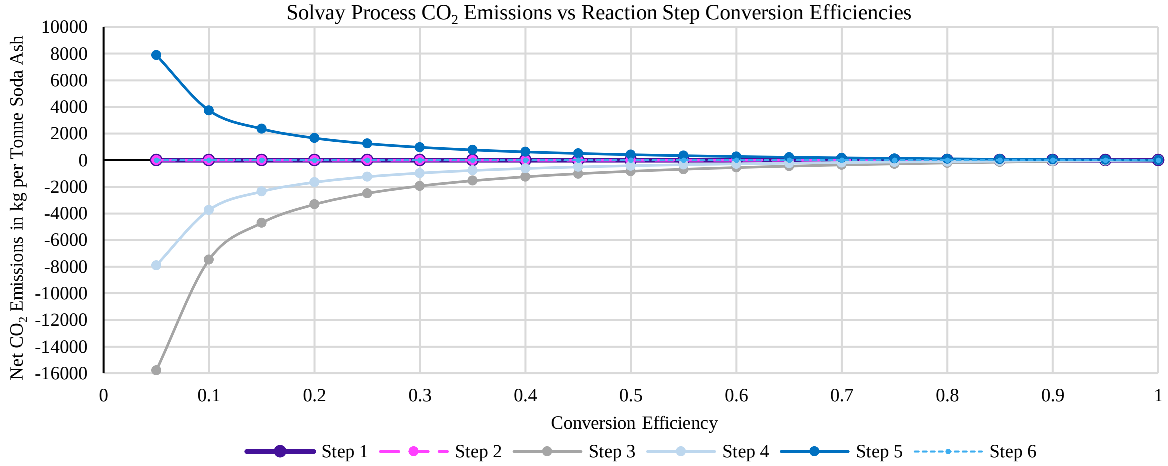


Figure 6-7 - Reaction step conversion efficiency vs maximum CO_2 uptake for the Solvay process.

Step 4 represents the calcination of $NaHCO_3$ to produce soda ash, CO_2 and water vapour. Consequently, lower conversion leads to reduced overall CO_2 emissions. However, in this event the energy and feedstocks will largely evade meaningful utilisation, resulting in significantly elevated OpEx; CapEx will also see inflation due to the larger process units required to match magnified upstream throughput. Conversion efficiencies at this step are typically very high; 85% conversion can be achieved via heating with low pressure steam, rising to 95% and 99% for medium and high-pressure steam respectively [282]. If the lower efficiency value of 85% is examined within the model data, 0.073 tonne CO_2 is up taken per tonne of soda ash. However, this comes with an associated 17% rise in limestone and sodium brine feed rates.

While reaction step 5 shows the potential to raise the net CO_2 emissions of the process, literature shows conversions of calcium oxide to calcium hydroxide can comfortably reach 95%-99% [283]. However, the efficiency is subject to factors such as the quality and purity of the calcium oxide, as well as quantity and temperature of the water used for slaking [284]. Using the lower bound of this range (95%), the model predicts a CO_2 emission rate of only 0.028 tonne per tonne soda ash. Consequently, the detrimental effects and associated concerns around low conversion in this step can be dismissed.

Examining the second process considered, the modified Solvay process (Figure 6-8), there is only one step through which reaction conversion efficiency can influence net CO_2 emission: the calcination of $NaHCO_3$ to soda ash. As noted for the Solvay process the step efficiency is typically >85%, meaning little deviation will be seen from the -0.415 kg CO_2 per kg soda ash observed at a uniform 100% conversion rate. At an 85% step 3 conversion an emission value of -0.562 tonne CO_2 per tonne soda ash is realised. However, this 35 % increase in stoichiometric CO_2 uptake is reflected through a 17.6% increase in required CaO and NaCl feed rates.

In contrasts to the traditional Solvay process, the chemistry of the modified version demonstrates a baseline net CO_2 uptake of 0.415 kg CO_2 per kg soda ash; a consequence of the carbonate group being generated via CDU as opposed to the calcination of limestone and the effective translation of its carbonate group through reactions. If a suitable CaO or $Ca(OH)_2$ source can be identified and utilised, this offers a significant advantage over the traditional process, reducing both complexity and CO_2 emissions.

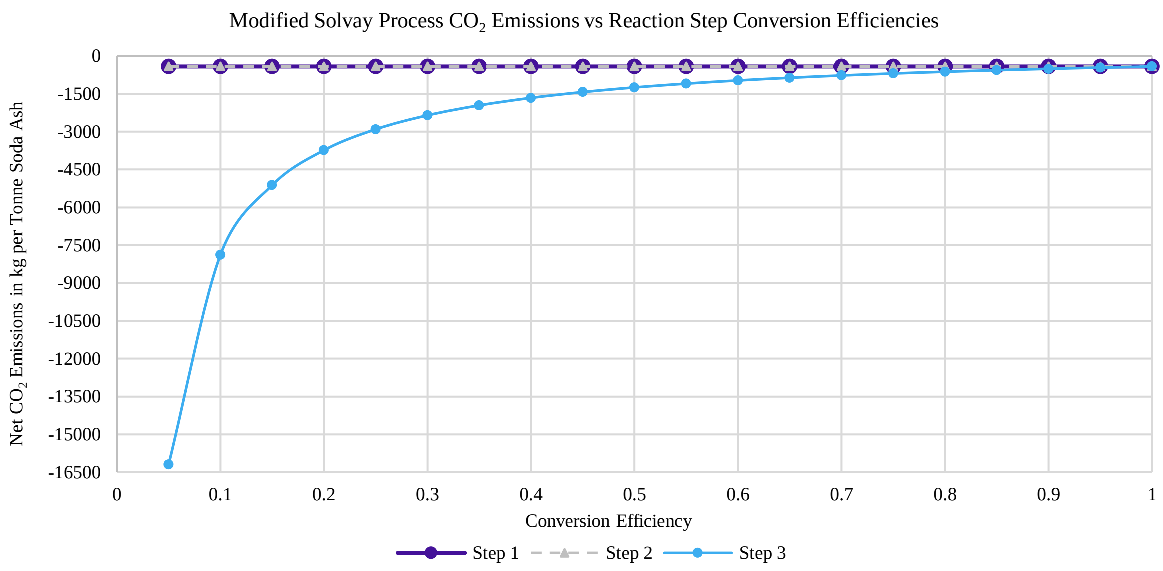


Figure 6-8 - Reaction step conversion efficiency vs maximum CO_2 uptake for the modified Solvay process.

Figure 6-9 details the behaviour of the Hou process. The absence of any emissive steps safeguards any performance benefits realised in other components of a larger value chain. In addition, step 3 and step 4 exhibit the largest CO_2 uptake, and therefore CDU, potential of any reaction across all three examined processes (16.2 tonne CO_2 per tonne soda ash).

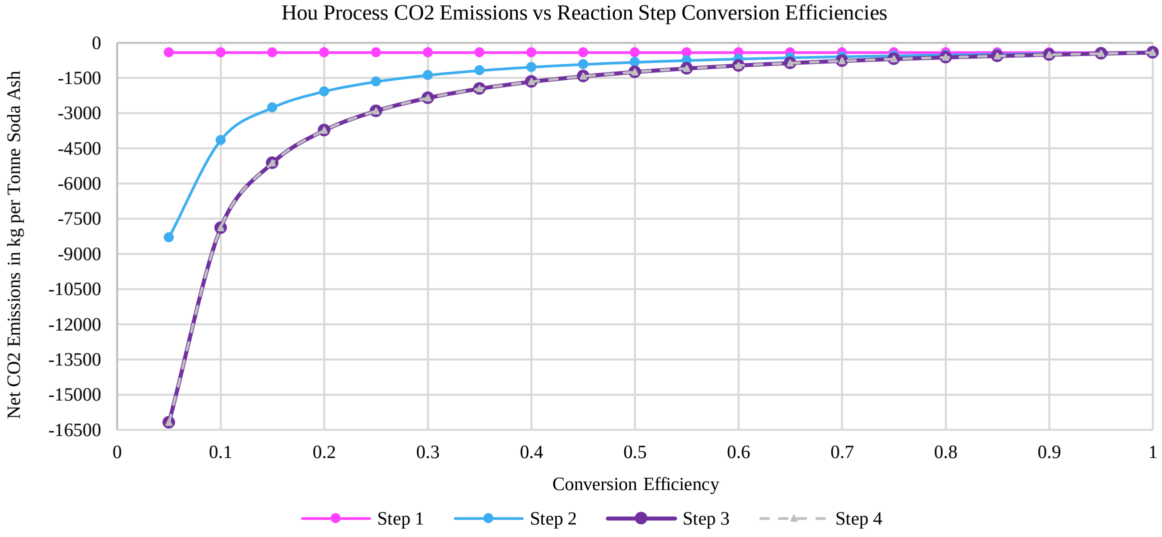


Figure 6-9 - Reaction step conversion efficiency vs maximum CO_2 uptake for the Hou process.

Step 4, the calcination of $NaHCO_3$ behaves identically to the corresponding step 3 of the modified Solvay process. However, in the Hou process, step 3 also exhibits the same CO_2 uptake behaviour, representing the generation of $NaHCO_3$ from NH_4HCO_3. Conversion below 100% at this step results in carbon leaving the process in the form of NH_4HCO_3. As discussed for the Solvay process, this results in the loss of ammonium ions; a problem exacerbated in the Hou process owing to its use in a potential co-product, ammonium chloride. Step 2 also offers elevated CO_2 uptake at lower conversions. However, as an intermediate step taking place within the carbonation tower, incomplete conversion leads to fed CO_2 leaving the process embedded in ammonium carbonate. Similarly to the modified Solvay process the Hou process' chemistry is carbon negative to the tune of 0.415 kg CO_2 per kg soda ash, again utilising fed CO_2 to form the soda ash's carbonate group. However, the Hou process offers three steps capable of CO_2 uptake as opposed to the modified Solvay's one.

6.4.4 Selection for Proof-of-Concept

Having evaluated the CDU potential of each process' chemistry, one must be selected for evaluation within the full hub and spoke assessment. Several criteria are specified to inform this decision;

1. Baseline CO_2 uptake at 100% conversion efficiency
2. Largest uptake potential (evaluated on the basis of a single reaction step)
3. Proportion of reaction steps offering CO_2 uptake potential

Quantified values for each process' performance against these criteria are calculated and specified in Table 6-11. While not a perfect method of selection, owing to the economically driven maximisation of the reaction step efficiencies, this decision must be made without the support of detailed LCAs from literature (evidenced by Section 6.3.2 and Table 6-5). Baseline CO_2 uptake is selected as a rough proxy for real-world post optimisation performance; higher stochiometric CO_2 utilisation can be seen as a strong indication of preferable deployment scenarios, at least when considering environmental impacts. Largest uptake potential is the weakest of the three criteria. However, it is included to evaluate the possibility of emission offsetting through the sequestration of CO_2 into secondary product, irrespective of their market value or utility. The proportion of reaction steps exhibiting CDU potential, the third and final criterion, is used to indicate how likely inefficiencies imposed by real world conditions and operation are to add or detract from net emission performance.

Table 6-11 – Selection criteria performance of processes considered for examination in the full proof-of-concept assessment.

Process	Selection Criteria		
	Baseline CO_2 Uptake (kg CO_2 / kg Soda Ash)	Largest Uptake Potential (kg CO_2 / kg Soda Ash)	Proportion of Steps Offering Uptake Potential (%)
Solvay	0	15.8	33.3
Modified Solvay	0.415	16.2	33.3
Hou	0.415	16.2	75

Consulting the criteria results, the Solvay process can immediately be dismissed, uniformly offering the least potential for CDU. The modified Solvay and Hou processes perform identically within the first two criteria; however, a clear divergence appears within the third. Where the Solvay and modified Solvay processes offer CDU potential in a third of the reaction steps, the Hou process elevates this to a lofty three quarters. On this basis, the Hou process is selected as the focus for a full proof-of-concept application of the hub and spoke framework.

This decision can be further buttressed by the consideration of several additional factors. Firstly, the modified Solvay process, the second most likely focus based on the evaluated criteria, has a significant weakness in the utilisation of a CaO or $Ca(OH)_2$ feed. Without abundant natural sources, their procurement is far from straightforward, likely relying on waste streams from other processes such as acetylene production [285]. Failing identification of such a source, a likely alternative is the pyrolysis of limestone, effectively resulting in a reversion to the traditional Solvay process.

In addition to this, the Hou process is typical of the CDU systems targeted for assessment by the hub and spoke framework. With Table 6-5 indicating that the Hou process has been the subject of very few existing studies, compounded by a general lack of openly available primary data, meaning the core difficulties associated with

CDU sustainability assessments are present; ultimately delivering a highly representative case study. The two studies that are present in existing literature are highly opaque and offer significantly divergent results for GWP (1.05 tonne CO_2 per tonne soda ash and 2.2 tonne CO_2 per tonne soda ash). Consequently, transparent evaluation of the system via the hub and spoke framework generates novel and valuable insights.

6.5 Goal and Scope Definition

The goal and scope of the proof-of-concept assessment are developed in alignment with the ISO 14k series standards [20], a requirement that underpinned many of the methodological decisions in Chapter 4. In the interest of transparency and ease of reference, the constituent requirements for each of these statements is provided in Table 6-12. Owing to the application of a novel framework, some of the aspects are approached in a slightly different way than traditional assessments; a notable example being the handling of assumptions. From this point onwards this chapter aims to validate and examine the workings of the developed methodologies.

Table 6-12 – Goal and scope statement requirements specified by ISO 14040

Component	Statement	
	Goal	Scope
Purpose	✓	
Application	✓	
Audience	✓	
Use in Comparative Assertions	✓	
Public Disclosure	✓	
Functional Unit		✓
System Boundaries		✓
Impact Categories		✓
Allocation Procedure		✓
Data Quality Requirements		✓
Type of Review (if any)		✓
Assumptions		✓
Limitations		✓

6.5.1 Goal

The purpose of this assessment is to act as a methodological proof-of-concept, examining and identifying near-future CDU value chain options for the production of soda ash via the Hou process in the APAC region. The targeted application is use within powdered laundry detergents for distribution and sale by Unilever Homecare in India. Through this, a broad range of value chain permutations are examined comparatively and ranked based on both objective performance against traditional indicators, and alignment to decision maker priorities regarding impact mitigation. Intended audiences include decision makers within Unilever and, where appropriate, their industrial partners.

6.5.2 Scope

The functional unit used within the assessment is one tonne of soda ash, assessed over a cradle-to-gate system boundary (see Figure 6-10). This excludes the transportation steps due to a lack of geographic specificity regarding the Hou process plant's location, a consequence of conducting an early-stage national-level resolution pathfinding assessment. Impact categories and indicators are selected across the environmental, economic, and societal assessment strands based on both usage frequency within existing works and relevance to the specific use case; the detailed selection processes and associated justification are laid out in Section 6.5.2.1. Allocation within the generation of feedstocks (spoke data sets) is handled on a mass basis in alignment with the prevailing Ecoinvent methodology [286]. Within the Hou process itself a co-product is generated in the form of ammonium chloride; however, it is unknown whether the market is of sufficient volume to seamlessly utilise the quantities generated. Consequently, a conservative approach is taken, and the impact burden is assumed to lie fully with the soda ash produced, representing a worst-case scenario. Data quality constraints are not specified due to the difficulties associated with the identification and verification of CDU process. However, all utilised data must be as temporally and geographically relevant as reasonably possible with the available system resolution; 2022 data is targeted due to improved availability and reporting completeness. The review process is substituted for a post-mortem of the methodological framework and SIA characterisation methodologies given that this assessment is intended as a proof-of-concept; within subsequent assessments this would be replaced with a sensitivity analysis. In a departure from standard assessment practices, assumptions will be detailed in the relevant hub and spoke LCI data sheets, this is necessary to facilitate the comparative assessments of all value chain permutations. Limitations are largely attributable to the lack of primary process data and geographic specificity; these will be discussed in more detail within the interpretation phase.

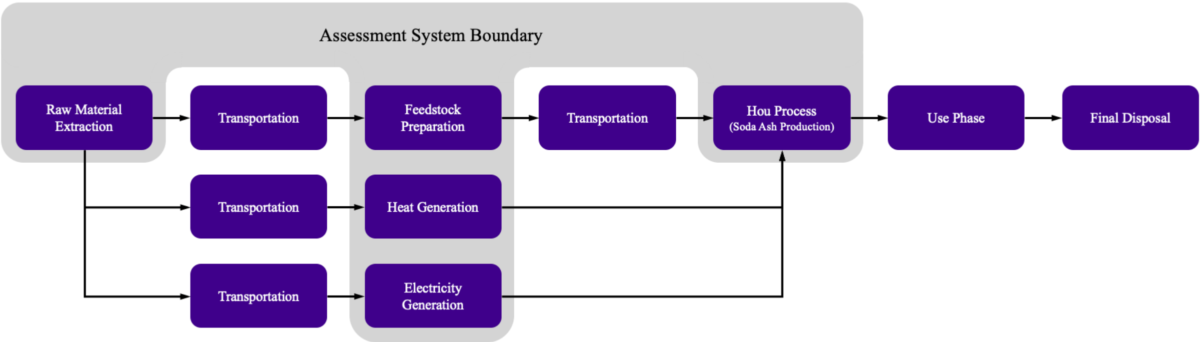


Figure 6-10 – Proof of concept assessment system boundary.

6.5.2.1 Impact Indicator and Characterisation Model Selection

Given the holistic nature of this framework and proof-of-concept, suitable impact indicators must be identified for each of the three strands. This task is therefore carried out independently on a strand-by-strand basis. Literature is consulted, in terms of both guidelines and existing assessments to determine the most commonly applied indicators where feasible. Indicators adding utility or supporting insight generation within the FMCG sector are also incorporated. In the case of the SIA strand, this selection is made to reflect the characterisation models developed in Chapter 5, acting as a validation study. These selected indicators are to be assessed relative to a local functional unit, specified for each hub or spoke set (as detailed in Chapter 4).

6.5.2.1.1 LCA Indicators and Characterisation Models

The hub and spoke framework has been developed to be as broadly applicable to FMCG value chain assessments as possible. However, Unilever, the FMCG company responsible for the commissioning of this work, have not mandated a set of desired indicators. Consequently, the environmental indicators for assessment are based on those recommended for consideration by existing guidelines. Table 6-13 details the guidelines consulted and their respective considered impact indicators. This is deemed to be a logical and systematic approach to indicator selection, keeping the total count within reasonable bound while ensuring inclusion of the most broadly relevant options.

Table 6-13 – LCA indicators suggested for assessment within major guidance documents.

Framework / Guideline	Observed LCA Impact Indicators																	
	Climate Change (GWP)	Ozone Depletion	Respiratory Inorganics	Ionizing Radiation	Acidification (Land)	Acidification (Water)	Acidification (Unspecified)	Eutrophication (Terrestrial)	Eutrophication (Freshwater)	Eutrophication (Marine)	Eutrophication (unspecified)	Ecotoxicity	Land Use	Resource Depletion (Abiotic)	Emissions to Water	Energy Consumption	Water Use	Particulate Matter
ILCD Handbook	✓	✓	✓	✓	✓	✓			✓	✓		✓	✓	✓				
BASF Eco-efficiency	✓	✓					✓						✓	✓	✓	✓		
BASF EEA6	✓	✓			✓	✓					✓			✓				
BASF EEA10	✓	✓			✓	✓					✓		✓	✓			✓	
CCaLC2	✓	✓					✓				✓						✓	
NETL	✓	✓									✓						✓	✓
PEF-CR	✓	✓		✓			✓	✓	✓	✓		✓	✓	✓			✓	✓

Examining this data, the most commonly applied indicators can be identified for subsequent utilisation within this study. While it is infeasible to manually assess the full suite of suggested indicators, a 'cut-off' frequency can be prescribed to select the most relevant. To this end, indicators appearing in more than three guidelines (≳43%) are adopted for this study.

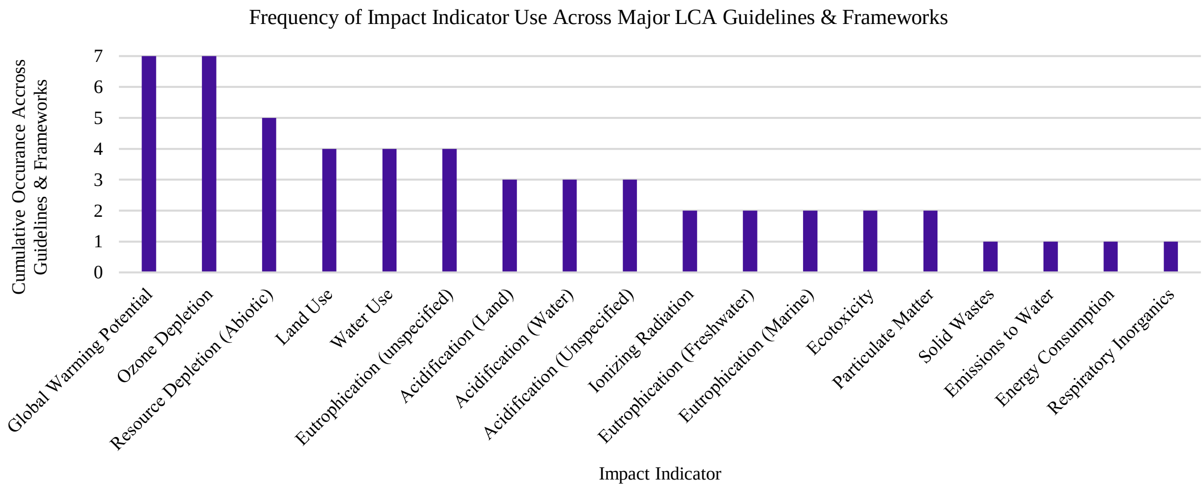


Figure 6-11 – Cumulative usage of common LCA impact indicators within widely recognised guidelines and frameworks

Some adjustments are made to this cut-off frequency based selection approach at the practitioner's discretion. Both marine and freshwater eutrophication are evaluated owing to the indicator's adoption by four guidelines on an unspecified basis. In contrast to this, acidification is only considered with respect to its terrestrial effects, reflecting scope constraints requiring the simultaneous assessment of a satisfactorily broad range of indicators in the TEA and SIA strands. Abiotic resource depletion can be assessed in terms of minerals, metals, or fossil fuels; a focus on mineral depletion is selected, reflecting its broad adoption and presence in ReCiPe's characterisation model offering [70]. Finally, land use is not considered as an LCA indicator due to its significant relevance to the societal assessment strand and developed characterisation models. This selection process delivers the indicators listed in Table 6-14.

Considering the selection of characterisation methods for use in the studies LCIA phase, two overarching impact pathway-oriented approaches are available, mid- and end-point. Of these options a mid-point evaluation is selected, owing to its ubiquitous presence in existing literature and greater insight delivery for practitioners. In addition, from a technical stance, mid-point indicators are more comprehensive, while also offering lower uncertainty; crucially for this work, they better facilitate the effective resolution of trade-offs across impact categories through the employment of weighting techniques, or more specifically, AHP-TOPSIS as selected in Chapter 4 [287]. With the general approach selected, the specific methods can be examined. Several candidates were previously identified in the literature review of Chapter 3, including but not limited to; CML2012, ReCiPe, TRACI 2.0, IPCC2013, Impact2002+, and USEtox. A primary goal of the selection process is to identify a broadly utilised method through which to evaluate compatibility with the hub and spoke framework. Consequently, a study was identified in literature that evaluates practitioners' preferences around the application of LCA characterisation methods [288]. This work consulted 145 LCA practitioners, of which 65% were active in the field on a weekly basis, to determine the most common characterisation practices. Results from the research are shown by Figure 6-12, clearly revealing ReCiPe to be the most favoured methodology (18.58% utilisation rate by consulted practitioners).

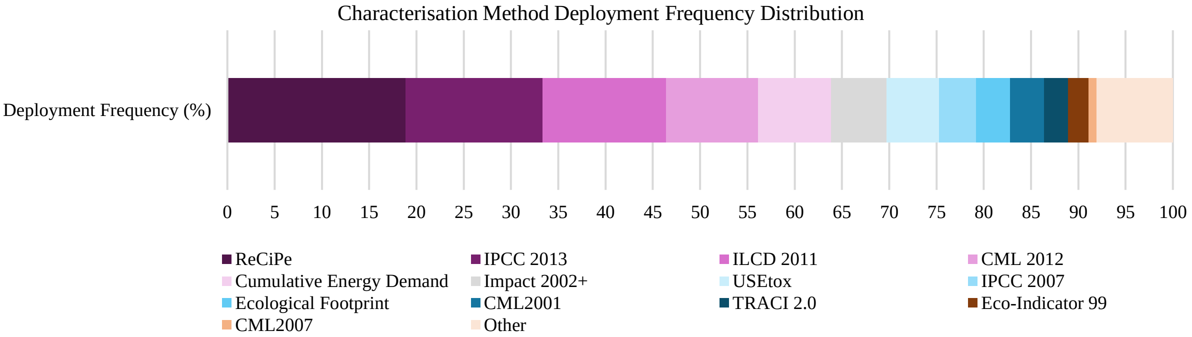


Figure 6-12 – Deployment frequency distribution of LCA characterisation methods by practitioners. Data is extracted from a literature study [288].

Interestingly, this conflicts with the advice given by GCI within their integrated LCA and TEA guidelines, in which CML's methods are recommended [39]. However, with no clear rationale laid out by the GCI for the selection of CML, this study will proceed with ReCiPe methodologies. This decision is taken to represent the modal application case, maximising the representativeness achieved by the proof-of-concept. The relevant ReCiPe characterisation methods [70] are identified for each of the previously selected LCA indicators and listed below in Table 6-14.

Table 6-14 – Impact indicators and characterisation methods selected for the proof-of-concept study's environmental strand. Where LFU is the local functional unit of the hub or spoke set being assessed.

Impact Indicator	Characterisation Method	Unit
Global warming potential	ReCiPe 2016 v1.1 (GWP 100 (Hierarchist))	kg CO_2-eq / LFU
Ozone depletion	ReCiPe 2016 v1.1 (ODP 100 (Hierarchist))	kg CFC11-eq / LFU
Mineral resource depletion	ReCiPe 2016 v1.1 (SOP (Hierarchist))	kg Cu-eq / LFU
Freshwater eutrophication potential	ReCiPe 2016 v1.1 (FETP (Hierarchist))	kg P-eq / LFU
Marine eutrophication potential	ReCiPe 2016 v1.1 (MEP (Hierarchist))	kg N-eq / LFU
Acidification potential	ReCiPe 2016 v1.1 (TAP (Hierarchist))	kg SO_2-eq / LFU
Water use	ReCiPe 2016 v1.1 (WCP (Hierarchist))	m3 / LFU

6.5.2.1.2 TEA Indicators and Characterisation Models

TEA indicators are less standardised than those observed in LCA [19]. In addition to this, there is a smaller pool of possible assessment indicators to choose from. Consequently, a less systematic, practitioner led approach is adopted. However, despite the resulting heavy reliance upon practitioner judgement, care is taken to ensure that the resulting indicator selection is both broad and of utility to FMCG companies such as Unilever. The result is the following list of TEA impact indicators;

- Capital expenditure (CapEx)
- Operational expenditure (OpEx)
- Mass efficiency
- Energy Efficiency
- Energy Demand

As discussed in Chapter 4's methodology development, CapEx is only evaluated for the hub process. As the only value chain step over which a FMCG company wields direct influence, it is also the only one for which they may feasibly need to put forward capital. In contrast to this, the OpEx is relevant across the full value chain. While its evaluation for spoke datasets will take the form of a market based purchase price estimate inclusive of the supplier's profit margins, the insight generation is of notable value and representative of value chain mechanics. Energy and mass efficiency are included to evaluate general performance and inform the FMCG company of any potential for continued improvement and optimisation around a given process. Energy demand is included due to its high influence on OpEx and feasibility-based capacity limitations. While energy demand and OpEx are typically correlated, energy prices can fluctuate significantly to alter the strength of this relationship, a pertinent example at the time of writing is the 163% rise in European industrial energy cost (per MWh and adjusted for inflation) between January 2021 and September 2022 [289]; a consequence of the Russian invasion of Ukraine and the associated oil and gas trading disruptions. In such high energy cost scenarios, OpEx may be effectively linearly related to energy demand.

Characterisation method selection for TEA also lacks the literature support seen around LCA. To ensure the adoption of a robust and repeatable approach, methodologies are identified from textbook and literature where possible. In cases where this is not possible an approach is specified and justified.

Table 6-15 - Impact indicators and characterisation methods selected for the proof-of-concept study's economic strand with the methodologies source, units, and relevant comments. Where LFU is the local functional unit of the hub or spoke set being assessed.

Impact Indicator	Characterisation Model Source	Unit	Comments:
Capital Expenditure (CapEx)	Sinnott and Towler [83]	£ (2022) / LFU	Prices adjusted to 2022 GBP using CEPCI
Operational Expenditure (OpEx)	Sinnott and Towler [83]	£ (2022) / LFU	Prices adjusted to 2022 GBP using CEPCI
Mass Efficiency	Mass balance	%	Based on the percentage yield relative to the product of interest (LFU)
Energy Efficiency	Weighted average of process unit heating efficiencies	%	Overview of the efficiency with which fuel and electricity is used. Based on literature efficiencies for considered unit or a comparable proxy.
Energy Demand	Energy balance	MJ / LFU	Based on summative estimates of the major unit's energy demand.

The selected CapEx characterisation method (focussing on the hub only) is based on the major process units within the hub process , as suggested by Sinnott and Towler [83];

> *"Capital cost estimates for chemical process plants are often based on an estimate of the purchase cost of the major equipment items required for the process, the other costs being estimated as factors of the equipment cost. The accuracy of this type of estimate will depend on what stage the design has reached at the time the estimate is made and on the reliability of the data available on equipment costs."*

These estimates are based on typical unit designs and adjusted based on size, throughput, and material [83], delivering the highest feasible degree of accuracy given the lack of primary data and pre-deployment assessment nature. Once these estimates are obtained for each unit, the costs are adjusted to 2022 GBP using the Bank of England's historical conversion rates and inflation adjuster [290] [291]. The Chemical Engineering Plant Cost Index (CEPCI) is also utilised to account for the difference in construction costs between the year examined by Sinnott and Towler (2009), and that of the assessment (2022); the utilised values are given in Table 6-16 and applied using Equation 6-1.

Table 6-16 – CEPCI values for the cost estimation year and assessment's year of focus [292]

Year	CPECI Values
2009	521.9
2022	816.0

Equation 6-1 – Application of the CEPCI values . Where, C is the estimated cost, and I is the CEPCI value for a given year (x and y).

$$C_{Year\,x} = C_{Year\,y} \times \frac{I_x}{I_y}$$

With the costs adjusted for CEPCI, inflation, and currency, Lang factors are applied to the purchase cost to account for; erection, piping, instruments, control systems, ancillary buildings, utilities, etc. The numerical values of these factors are given in Table 6-17 based on the process type examined. The sum of these factors for the relevant process type is then used to scale the time, currency, and CEPCI adjusted equipment cost, delivering the total estimated CapEx for the plant.

Table 6-17 – Lang factors for use in CapEx estimation. Values are extracted from Sinnott and Towler [83]

Lang Factors			
Consideration	Process Type		
	Fluids	Fluids - Solids	Solids
Equipment Erection	0.4	0.45	0.5
Piping	0.7	0.45	0.2
Instrumentation	0.2	0.15	0.1
Electrical	0.1	0.1	0.1
Buildings	0.15	0.1	0.05
Utilities	0.5	0.45	0.25
Storages	0.15	0.2	0.25
Site Development	0.05	0.05	0.05
Ancillary Buildings	0.15	0.2	0.2
Design and Engineering	0.3	0.25	0.2
Contractor's Fee	0.05	0.05	0.05
Contingency	0.1	0.1	0.1

This derived CapEx value is for the plant and does not consider a study's functional unit (or hub local functional unit). In order to evaluate the CapEx relative to the functional unit, the throughput of the plant over its full lifetime must be known. For this proof-of-concept study, a typical soda ash plant throughput of 164,000 tonnes per annum is identified in literature, with an estimated operational lifetime of 30 years [256]; yielding 4,920,000 tonnes of soda ash in total. The projected CapEx from Equation 6-1 and Table 6-17 must therefore be divided by this total to deliver a CapEx contribution per functional unit.

OpEx is much more straightforward to evaluate. For each of the hub and spoke LCI's, market prices are evaluated for all feedstocks and utilities consumed per local functional unit, representing the evaluated technology route and location. These values are adjusted for inflation and currency in the same manner as the unit costing in the CapEx methodology [290] [291]. Where possible, the market prices should be identified for the specific country of operation. However, where this is not possible, an average for a larger geographic region can be used, provided this is noted within the hub or spoke's data sheet as an assumption and limitation. The detail of the calculation approaches adopted for mass and energy efficiency, as well as total energy demand are given in Table 6-15, and can be seen in more detail within each of the hub and spoke datasheets within Appendix C.

6.5.2.1.3 SIA Indicators and Characterisation Models

The selection of SIA indicators is, in this case, the most straightforward of the three strands. Chapter 5's seven indicators and associated characterisation models will be adopted within the proof-of-concept study. This builds upon McCord *et al.*'s [7] modification of the UNEP and SETAC suggested stakeholder groups, generating a quantified and repeatable FMCG and CDU specific approach to social assessments. The indicators to be assessed, covering the UNEP and SETAC stakeholder categories of workers and the local community, are therefore;

- Risk of forced labour
- Risk of child labour
- Risk of change in access to electricity
- Risk of change in access to water
- Risk of land use change
- Occupational safety and health
- Utilisation of hazardous materials

A more detailed description of the semi-systematic indicator selection process was outlined in Chapter 5 prior to the development of characterisation methods. Their assessment within this proof of concept will facilitate examination of the characterisation method's performance, value addition, and influence on value chain recommendation to the FMCG company.

6.5.2.1.4 Indicator and Characterisation Method Overview

To summarise the selection of indicators for this proof-of-concept study, a broad range has been selected, covering the three strands of sustainability. The LCA strand's have been systematically chosen to deliver a highly representative set, including the most commonly deployed indicators and characterisation models used by practitioners (see Figure 6-11 and Figure 6-12 respectively). Such a selection will verify that the developed hub and spoke framework is fit for broader application within the field of sustainability assessment.

The TEA indicator selection was the least systematic of the three strands, selected based on Unilever PLC's requirements and general applicability to FMCG oriented assessments. Characterisation methods employed include a range of published methodologies (OpEx and CapEx), and mass and energy balance based evaluations (efficiencies and energy demand). SIA's selection strategy was adopted from Chapter 5, focussing on the UNEP and SETAC guidelines, and more specifically, their use within CDU relevant applications such as those seen in this study. Due to their thorough consideration within the previous work, the selection process or rational was not repeated in its entirety. The resulting indicator selection, representing the final constituent component of the assessment's scope, delivers the aggregated super-set given in Table 6-18.

Table 6-18 – Final holistic indicator selection and their units for each assessment strand.

Assessment Strand:	Indicator:	Units:
LCA	Global Warming Potential	kg CO_2-eq / LFU
	Ozone Depletion	kg CFC11-eq / LFU
	Mineral Resource Depletion	kg Cu-eq / LFU
	Freshwater Eutrophication Potential	kg P-eq / LFU
	Marine Eutrophication Potential	kg N-eq / LFU
	Acidification Potential	kg SO_2-eq / LFU
	Water Use	m^3 / LFU
TEA	CapEx	MJ / LFU
	OpEx	2022 £ / LFU
	Mass Efficiency (%)	%
	Energy Efficiency (%)	%
	Energy Demand	2022 £
SIA	Forced Labour	-
	Child Labour	-
	Risk of Change in Access to Water	-
	Risk of Change in Access to Electricity	-
	Risk of Land Use Change	-
	Occupational Health and Safety (OSH)	-
	Utilisation of Hazardous Materials	-

6.6 Framework Application

With the goal and scope fully defined, the application of the hub and spoke framework can begin. This clearly requires several key initial considerations; the identification of spoke processes for evaluation, configuration of the MCDM value choice inputs, LCI generation strategy, and LCIA approach.

6.6.1 Spoke Process Selection

The Hou process, selected in Section 6.4 as the hub for the proof-of-concept assessment, has several inputting boundary flows. As a consequence of the cradle-to-gate assessment scope, the post-production impact of the soda ash within powdered laundry detergent is not evaluated. Furthermore, the direct emissions from the Hou process are handled uniformly across all scenarios and evaluated within the hub's LCI, therefore not requiring gaseous emission, liquid effluent, and solid waste spokes. This leaves the consideration of the process inputs as the basis of spoke sets, representing the upstream value chain:

- Sodium Brine (NaCl)
- Ammonia (NH_3)
- CO_2
- Electricity
- Heat

When selecting the constituent spokes for a proof-of-concept, it is important to ensure that there is a mixture of set sizes; delivery of this ensures that a range of framework application scenarios examined. Upper bounds for set size must be cognisant of time constraints, requiring data collection and LCI generation for each. However, nor should the sets be so small as to prevent meaningful comparison and local performance based normalisation. Consequently, sets of sizes between 5 and 9 are targeted. Spoke identification is also subject to literature availability, again recognising the FMCG mandated deployment ready focus of the assessment and associated time constraints. In addition to these factors, a diverse range of technology types is desirable, delivering differentiated performance profiles and aiding evaluation of the framework's efficacy. The result of these considerations is shown in Table 6-19. China is added as a secondary option for most feedstock routes; a decision taken previously to reflect the close geographic proximity to India, and their significant industrial capacity.

As detailed in Section 4.5.3.7, the spokes used in the proof-of-concept assessment are identity tagged using a decimal system comprising of two numbers, the first identifying the spoke set and the second the specific spoke. The final identification convention and the included processes and technologies are outlined in Table 6-19.

Table 6-19 – Spoke sets and their constituents selected for assessment within the proof-of-concept study.

Spoke Sets	Spokes	I.D.
Ammonia (NH_3)	SMR HB (India)	1.1
	SMR HB (China)	1.2
	PEM (Wind) eHB (India)	1.3
	PEM (Wind) eHB (China)	1.4
	PEM (Grid) eHB (India)	1.5
	PEM (Grid) eHB (China)	1.6
	PEM (Grid) eHB (Germany)	1.7
	Biogas SMR HB (India)	1.8
	Biogas SMR HB (China)	1.9
Sodium Chloride (NaCl)	Direct Solution Mining (India)	2.1
	Direct Solution Mining (China)	2.2
	Indirect Solution Mining (India)	2.3
	Indirect Solution Mining (China)	2.4
	Rock Salt Mining (India)	2.5
	Rock Salt Mining (China)	2.6
Carbon Dioxide (CO_2)	DAC (India)	3.1
	DAC (China)	3.2
	DAC (Germany)	3.3
	MEA (India)	3.4
	MEA (China)	3.5
Electricity	Wind (India)	4.1
	Solar (India)	4.2
	Bioenergy (India)	4.3
	Hydro (India)	4.4
	CHP, Lignite (India)	4.5
	CHP, Oil (India)	4.6
	CHP, Biogas (India)	4.7
	CHP, Natural Gas (India)	4.8
	Grid (India)	4.9
Heat	CHP, Lignite (India)	5.1
	CHP, Oil (India)	5.2
	CHP, Biogas (India)	5.3
	CHP, Natural Gas (India)	5.4
	Natural Gas, Furnace (India)	5.5
	Biomass, Furnace (India)	5.6

6.6.2 MCDM Configuration

In this first application case, it is decided that the MCDM inputs should be left uniform and unaltered by decision maker value choices. This delivers identical weightings for all indicators listed in Table 6-18. While it is important to recognise that this is, in itself, a subjective methodological choice, it offers the best platform from which to evaluate the framework's mechanics and outputs. Furthermore, this approach gives a consistency ratio of one (CR = 1) for each of the four scoring matrices, eliminating any data artifacts attributed to minor input inconsistencies. The impact of the MCDM inputs on the framework's value chain recommendation (spoke selection preferences) will be examined in isolation and rank reversal observations explored and discussed in Section 6.7.6. A screenshot of the models MCDM configuration for the proof-of-concept study is shown by Figure 6-13. Taking this approach, each of the 19 indicators receive a weighting of 0.05263.

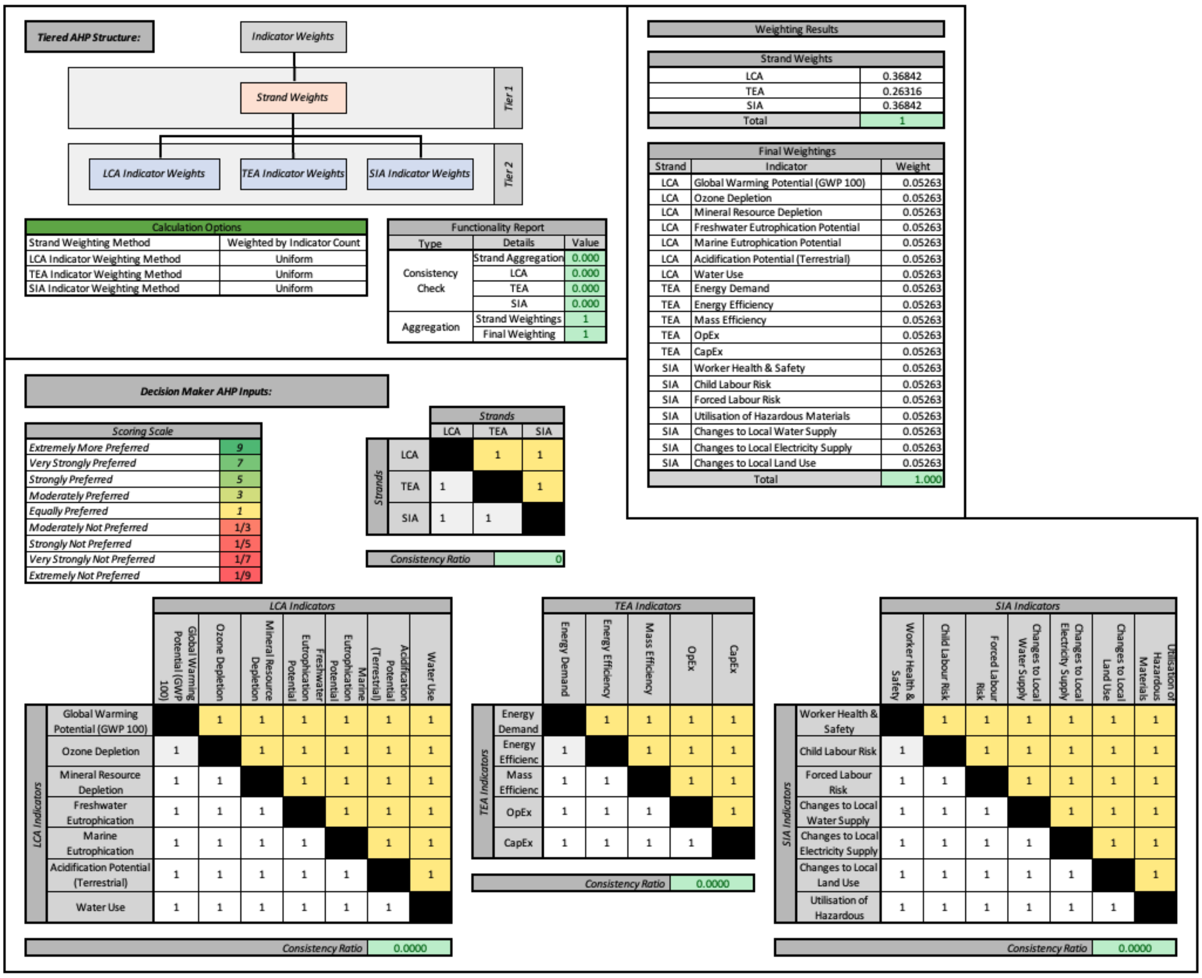


Figure 6-13 – Framework tool MCDM configuration for the proof-of-concept study.

6.6.3 Lifecycle Inventory Generation

Literature search findings and LCI generation cannot be evaluated for all spokes within the thesis, a consequence of length restrictions. However, a general procedure will be specified with an example presented for grid mix impacts. Grid electricity supply LCA / LCI data was selected as the demonstration case as is pertinent to all hubs and spokes, therefore maximising the relevance. Each of the other spoke's data sheets can be seen in the supplementary material (Appendix C), including all system boundaries, mass balances, and assumptions utilised.

Within the spoke data sheets, the processes that directly feed the Hou process, or hub, are modelled as the foreground system with constituent unit operations considered independently. Tertiary systems or processes such as mining or plant construction are treated as the background system with Ecoinvent v3.8 data sets providing the LCI data. EcoQuery is used to return data sets for the required intermediate flows (between the foreground and background systems) while reflecting the spatial, temporal, and technological scenarios as accurately as possible. Where perfectly representative data is not available, the closest alternative is utilised and noted in the relevant datasheet. Validity of the modelled systems' mass balances is confirmed by checking for conservation of mass across both the whole system, and each constituent major unit operation (excluding heat exchangers, pumps, etc.).

6.6.3.1 Electricity & Grid Mix Data

The examination of national grid impacts is, as previously noted, used as the example case for spoke set LCI generation. Given the broad range of applications targeted by the framework, grid impacts will be evaluated for as many countries as possible. This also allows for consideration of a wider range of spoke options (geographically) beyond India within the proof of concept. Furthermore, the consideration of a wide range of countries grid mixes offers an opportunity to test and demonstrate interoperability within the framework, generating a set of spokes that can be re-used on a 'plug and play' basis.

6.6.3.1.1 General Approach

To quantify the impacts associated with national level electricity production, two supporting data sets must be defined;

1. The fractional contributions of generation sources to national grids
2. Each generation sources impact profile (considering LCA for this example).

Subsequent aggregation of these data sets allows for the calculation of impact indicator values per kWh of supplied electricity in each country (Figure 6-14). The selection of lifecycle steps for inclusion, such as plant construction, is informed by a sensitivity analysis outlined in Section 6.6.3.1.3.

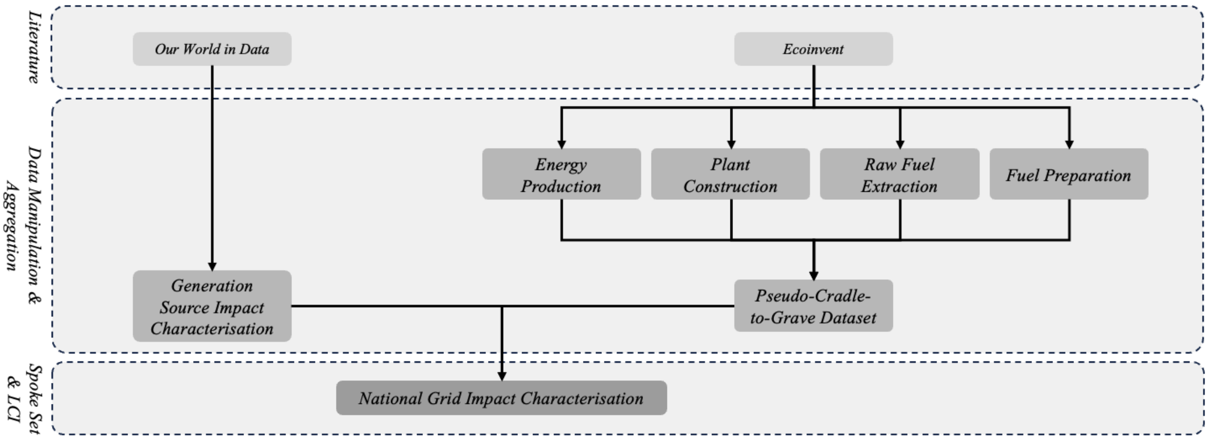


Figure 6-14 – Data extraction strategy for the characterisation of environmental impacts associated with electricity generation.

6.6.3.1.2 Identification and Handling of Grid Mix Composition Data

The first of the data sets, the national grid compositions, is derived from literature data [293]. Data collection from a single source was targeted to ensure consistent peripheral methodologies; the reported values can be traced back to a set of Ember 'Energy Institute Statistical Review of World Energy' [294] reports published in July 2023. In total, this delivers grid compositions for 206 countries. This national-level granularity successfully achieves alignment with the larger proof-of-concept assessment's scope. Ecoinvent (ReCiPe (H) Midpoint) is used to quantify each electricity generation source's impact indicator values, assuming globally comparable energy generation technologies based on current BAT (i.e. energy generation plants have comparable performances irrespective on country of operation). While this represents a limitation of the study, the variation in each generation source's performance is expected to be relatively insignificant on a national level. The data extracted from literature provides grid mixes in the form of kWh per capita year across nine distinct generation sources. Equation 6-2 is employed to convert these into percentage shares.

Equation 6-2 – Calculation of total grid mix share supplied by a given generation source

$$Percentage\ grid\ share\ (GS)\ of\ generation\ source\ i\ = \frac{National\ energy\ derived\ from\ generation\ source\ i\ \left(\frac{kWh}{capita\ year}\right)}{Total\ National\ Energy\ Use\left(\frac{kWh}{capita\ year}\right)}$$

Subsequently, a grid share matrix is compiled, detailing generation source production shares and country. Figure 7-10 shows the matrix structure, where the numerical subscript indicates the country, and the letter indicates the generation source. The result is the full definition of 206 countries' grid mixes as a function of the nine-generation sources, ensuring granularity matching that of the SIA characterisation models developed in Chapter 5.

$$\begin{matrix} GS_{1a} & GS_{1b} & \dots \\ GS_{2a} & GS_{2b} & \dots \\ \dots & \dots & \dots \end{matrix}$$

Figure 6-15 – Format of grid mix composition matrix. Where, numerical subscripts denote country considered, and alphabetical subscripts indicate the generation method.

Due to the size of the data set, it is not feasible to tabulate grid mix composition for all 206 countries within this thesis. Consequently, the G20 nations are displayed within Table 6-20 as an example set for use in later data analysis, using the LCI format shown in Figure 6-15. This G20 grid mix data omits the EU as all constituent nations are examined independently within the full data set, adhering to the desired national level resolution.

Table 6-20 – Grid mix compositions for the G20 nations.

Country	Generation Source Grid Mix Share (%)								
	Coal	Gas	Oil	Nuclear	Hydro	Wind	Solar	Bioenergy	Other Renewables
Argentina	1.90	60.67	5.15	6.93	13.76	8.73	1.48	1.37	0.00
Australia	51.32	17.79	1.76	0.00	5.97	10.56	11.35	1.25	0.00
Brazil	3.81	13.74	3.47	2.22	54.76	10.79	2.53	8.69	0.00
Canada	5.88	11.55	0.44	13.96	60.25	5.63	0.82	1.47	0.00
China	62.93	3.21	0.14	4.80	15.32	7.73	3.85	2.00	0.00
France	0.99	6.06	1.79	68.93	10.83	6.69	2.86	1.74	0.11
Germany	28.30	16.38	3.73	11.89	3.38	19.72	8.49	8.07	0.04
India	74.17	3.75	0.13	2.56	9.36	3.97	3.99	2.07	0.00
Indonesia	61.40	18.27	2.15	0.00	7.98	0.14	0.06	4.84	5.14
Italy	4.90	50.28	4.20	0.00	15.85	7.31	8.74	6.66	2.06
Japan	32.51	35.12	3.37	6.39	8.26	0.93	9.25	3.85	0.32
Mexico	3.94	59.18	9.55	3.39	10.23	6.22	4.20	2.01	1.27
Russian Federation	17.30	41.99	0.72	20.03	19.32	0.35	0.21	0.04	0.04
Saudi Arabia	0.00	60.55	39.22	0.00	0.00	0.00	0.23	0.00	0.00
South Africa	86.35	0.00	0.65	5.44	0.66	3.75	2.98	0.18	0.00
Korea, Rep.	35.72	29.76	1.18	25.58	0.52	0.54	4.07	2.57	0.08
Turkiye	30.48	33.35	0.62	0.00	16.78	9.43	4.18	1.93	3.24
United Kingdom	1.93	40.23	2.79	15.26	1.82	21.17	4.06	12.73	0.00
United States	21.62	38.02	0.85	18.77	5.93	9.11	3.96	1.31	0.44

6.6.3.1.3 Energy Generation Source Impact Assessment

Having determined the required nation grid mixes, the impacts of each generation source must be quantified. To facilitate integration with the national grid mix data set, these will be examined on the basis of a 1 kWh functional unit. The following nine sources were reported as present in the literature for national grid compositions [293];

- Coal
- Oil
- Natural gas
- Nuclear
- Hydroelectric
- Wind
- Solar
- Bioenergy
- Other Renewables

The composition of the final source, 'other renewables', is not clearly specified within the utilised dataset [293]. Consequently, its impacts will be represented by an average of the values delivered by hydroelectric, wind, and solar sources. In the analysis, wind energy is assumed to be generated via an even proportion of on-shore and off-shore installations. This results in the selection of the following Ecoinvent 3.8 datasets, representing the nine generation sources (Table 6-21).

Table 6-21 – Ecoinvent v3.8 unit datasets selected for the characterisation of assessed electricity generation methods.

OWID Generation Source	Production Route / Data Set Used	Justification for Selection
Coal	'electricity production, hard coal - electricity, high voltage'	The dataset offered a match for the generation route.
Natural Gas	'electricity production, natural gas, combined cycle power plant - electricity, high voltage'	The combined cycle plant was selected as it is the most representative technology globally [295].
Oil	'electricity production, oil - electricity, high voltage'	The dataset offered a match for the generation route and was the only oil-based energy generation dataset within Ecoinvent 3.8.
Nuclear	'electricity production, nuclear, pressure water reactor - electricity, high voltage'	PWRs are the most common type of reactor in operation globally [296], with 300 in use.
Hydroelectric	'electricity production, hydro, run-of-river - electricity, high voltage'	Run-of-river (also called impoundment) is the most common method of hydroelectric energy generation [297].
Wind (Averaged)	'electricity production, wind, 1-3MW turbine, onshore - electricity, high voltage'	A majority of installations state a nameplate capacity of 2.5-3MW [298]
	'electricity production, wind, 1-3MW turbine, offshore - electricity, high voltage'	Most installations have a nameplate capacity of >3MW [298]. However, the largest capacity dataset available on Ecoinvent 3.8 is 1-3MW.
Solar	'electricity production, solar tower power plant, 20 MW - electricity, high voltage'	Represents the only solar energy generation source available in Ecoinvent 3.8.
Bio Energy	'heat and power co-generation, wood chips, 6667 kW - electricity, high voltage'	The dataset offered a close match for the generation route and was the only biomass-based energy generation dataset with the correct reference product within Ecoinvent 3.8.
Other Renewables	Aggregate (Hydroelectric, Wind, & Solar)	Taken as an average of hydroelectric, wind, and solar impact indicator values. The grid mix data set from literature do not specify the nature of 'other renewables'.

The datasets were examined to determine their system boundaries, revealing a gate-to-gate scope. Consequently, a broader network of data sets must be aggregated to obtain the cradle-to-gate insights required within the proof-of-concept. However, this introduces a question about the required extent and resolution of data collection required to be representative of real impacts. In response to this, reporting completeness studies were conducted to determine which lifecycle stages contributed significantly to environmental impacts, requiring inclusion in the full proof-of-concept LCIs. The employed approach is outlined now using electricity generation impacts as an example. The environmental strand was selected for this demonstration as it is directly affected by the resulting decision; OpEx data is based on purchase price per kWh which remains constant irrespective of boundary definition, and SIA is carried out on a geographic basis resulting in similar independence from the system boundary specification.

1 kWh of fuel oil-derived electricity is to be examined as the reference product, applying several system boundary configurations, and examining the resulting impacts on reporting completeness. Oil based electricity, selected for evaluation due to its position as the most common generation source globally (30.9%) [299], was examined through the aggregation of Ecoinvent 3.8 datasets. To link these constituent sets, a tree diagram was created (see Figure 6-16), where the green value denotes the reference product (1 kWh), and the red values show the intermediate flows between datasets. The impacts contributed by each of the datasets (unit operations) are calculated as the product of the impact per local functional unit and the cascade multiplier (the product of all intermediate flows on the shortest path to the reference product).

The total impact of this network (boundary 3) is examined against the seven indicators selected for the proof-of-concept study. With these values quantified as a 'complete' (baseline) impact analysis, a comparison can be drawn with the results returned by boundary 1 and boundary 2 (Figure 6-16).

Table 6-22 – Summary of reporting completeness for different proposed system boundaries.

Indicator	Unit	Objective Results	Reporting Completeness (%)		
			Boundary 1	Boundary 2	Boundary 3
Global Warming Potential (GWP 100)	kg CO_2-eq / kWh	1.14	99.212	99.946	100
Ozone Depletion	kg CFC11-eq / kWh	6.23×10^{-7}	99.762	99.995	100
Mineral Resource Depletion	kg Cu-eq / kWh	1.85×10^{-2}	94.828	95.762	100
Freshwater Eutrophication Potential	kg P-eq / kWh	3.52×10^{-5}	100	100	100
Marine Eutrophication Potential	kg N-eq / kWh	1.73×10^{-3}	99.582	99.992	100
Acidification Potential (Terrestrial)	kg SO2-eq / kWh	9.42×10^{-3}	99.395	99.990	100
Water Use	m3 / kWh	1.12×10^{-3}	99.191	99.999	100

Examining the three sets of reporting completeness results (Table 6-22), boundary 1 is seen to capture an average of 98.85% of the total impacts of the system across all seven indicators. However, the coverage is <95% complete for the mineral resource depletion indicator. However, in contrast to the mineral resource depletion, the other six indicators exceeded 99% reporting completeness for both boundary 1 and 2, suggesting very low sensitivity to system boundary's location beyond the generation step. On balance, boundary 2 may be a better fit for the evaluation of the nine energy generation sources, surpassing the 95% reporting completion in all indicators. It is recognised that the exact reporting completeness for a given approach to boundary setting will vary with technology type and generation source. For instance, the construction phase is more likely to have a higher share of impact contributions for solar (very low operating emissions) than a fossil-based plant with significant operational emissions.

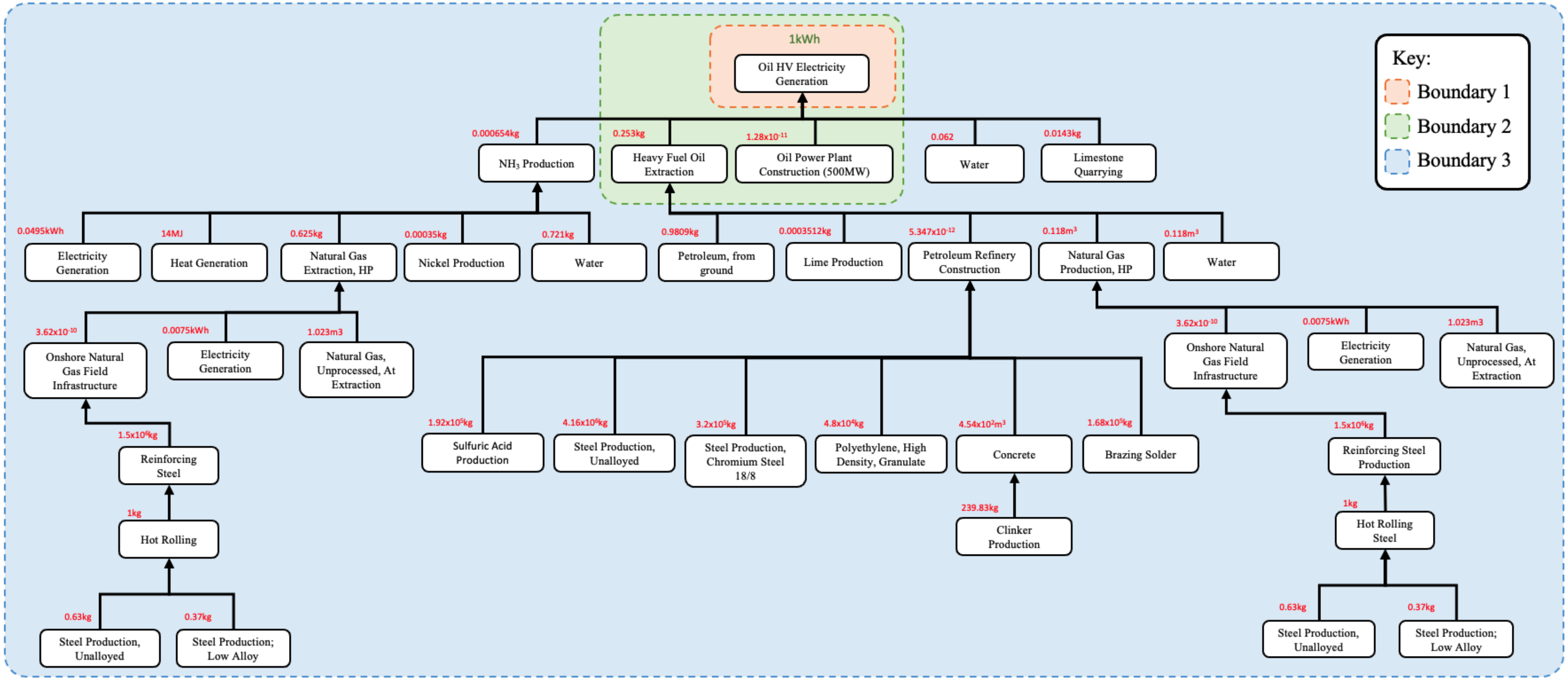


Figure 6-16 – System boundaries considered in the selection of cut-off criteria for the setting of subsequent spoke data sets.

This data can alternatively be viewed in the context of the cascade multiplier, showing the drop off in reporting completeness visually (Figure 6-17). Use of this approach removes the rigid rules around activity inclusion within the system boundary, choosing to instead base inclusion on the magnitude of each value chain step's relative contribution. The results in Figure 6-17 mirror the conclusions drawn from the three system boundaries in Table 6-22, highlighting the sensitivity of mineral resource depletion reporting completeness. However, additional insights are delivered, showing that activities with cascade multipliers above 0.3 dominate impact reporting due to their flow magnitudes.

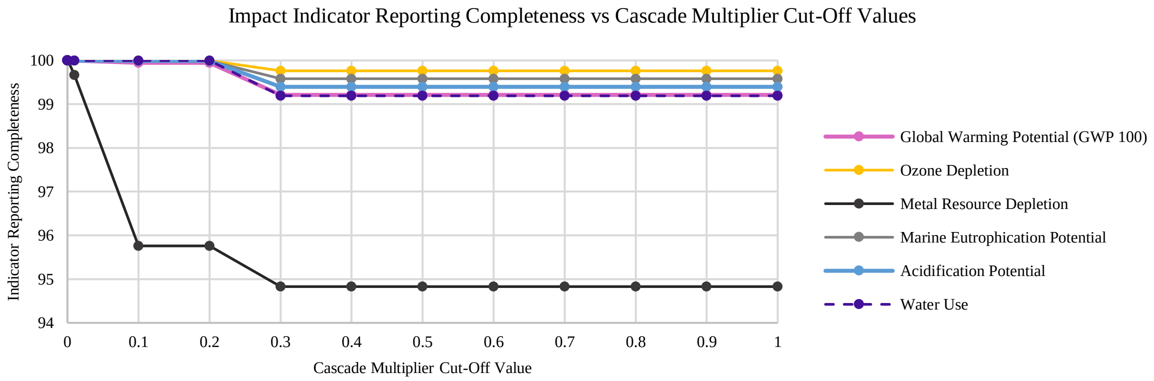


Figure 6-17 – Reporting completeness based on application of the cascade multiplier as a system boundary cut-off criteria.

Despite this case study, and both data formats (Figure 6-17 and Table 6-22), demonstrating the dominance of the primary gate-to-gate energy generation dataset over the cradle-to-gate lifecycle impacts of boundary 3, it was decided that four datasets should be aggregated to quantify the 1 kWh's pseudo-cradle-to-gate impact profile for each generation source; they reflect the constituents of boundary 2 and their natures are detailed in Table 6-23. Additionally, the aggregation procedure for the datasets is given by Equation 6-3. The incorporation of a fourth dataset beyond the three included within boundary 2 (fuel extraction) ensures that the impacts associated with non-fossil generation sources are also captured effectively and fairly. Where renewable generation source's impacts primarily reside within the construction phase, fossil alternatives rely on resource extraction and refining that must be included in the system boundary to deliver parity in reporting completeness.

Table 6-23 – Notation used for the system boundary components included within the assessment of electricity generation.

Lifecycle Phase	Notation
Energy Production	LP_1
Plant Construction	LP_2
Raw Fuel Extraction	LP_3
Fuel Preparation	LP_4

Equation 6-3 – Calculation of impact indicator results for each generation source considered.

$$Generation\ Source\ Indicator\ n\ Value = \sum_{i=1}^{4} (LP_i\ indicator\ n\ value\ per\ reference\ product \times LP_i\ reference\ flow)$$

With the lifecycle phases for consideration specified, corresponding datasets can be extracted from Ecoinvent 3.8. Table 6-24 shows the final selection for each of the generation sources. For renewable routes, some datasets may be absent owing to the burden-free availability of the 'fuel' (wind, run-of-river, and solar radiation). The resulting overall impact indicator results for the electricity generation types are given in Table 6-25 as calculated via Equation 6-3.

Table 6-24 – Overview of the data sources and intermediate flows utilised in the assessment of electricity generation impacts.

OWID Generation Source	Lifecycle Phase	Ecoinvent v3.8 Dataset Used	Intermediate Flow (per kWh)
Coal	Energy Production	'electricity production, hard coal - RoW - electricity, high volt	1
	Plant Construction	'hard coal power plant construction, 100MW - GLO - hard coal power plant'	$1.33x10^{-11}$
	Raw Fuel Extraction	'hard coal mine operation and hard coal preparation - RoW - hard coal'	0.439
	Fuel Preparation		
Natural Gas	Energy Production	'electricity production, natural gas, combined cycle power plant - RoW - electricity, high voltage'	1
	Plant Construction	'gas power plant construction, combined cycle, 400MW electrical - RoW - gas power plant, combined cycle, 400MW electrical'	$1.39x10^{-11}$
	Raw Fuel Extraction	'natural gas production, unprocessed, at extraction - GLO - natural gas, unprocessed, at extraction'	0.186
	Fuel Preparation	'natural gas production - RoW - natural gas, high pressure'	0.185
Oil	Energy Production	'electricity production, oil - SI - electricity, high voltage'	1
	Plant Construction	'oil power plant construction, 500MW - RoW - oil power plant, 500MW'	$1.87x10^{-11}$
	Raw Fuel Extraction	'petroleum production, onshore - RoW - petroleum'	0.360
	Fuel Preparation	'heavy fuel oil production, petroleum refinery operation - RoW - heavy fuel oil'	0.367
Nuclear	Energy Production	'electricity production, nuclear, pressure water reactor - RoW - electricity, high voltage'	1
	Plant Construction	'nuclear power plant construction, pressure water reactor, 1000MW - RoW – nuclear'	$3.22x10^{-12}$
	Raw Fuel Extraction	'uranium fuel element production, enriched 4.2%, for light water reactor - RoW - uranium, enriched 4.2%, in fuel element for light water reactor'	$2.26x10^{-6}$
	Fuel Preparation	'nuclear fuel element production, for pressure water reactor, UO2 4.2% & MOX - RoW - nuclear fuel element, for pressure water reactor, UO2 4.2% & MOX'	$2.46x10^{-6}$
Hydroelectric	Energy Production	'electricity production, hydro, run-of-river - RoW - electricity, high voltage'	1
	Plant Construction	'hydropower plant construction, run-of-river - RoW - hydropower plant, run-of-river'	$8.07x10^{-13}$
	Raw Fuel Extraction	N/A	N/A
	Fuel Preparation	N/A	N/A
Wind (Onshore)	Energy Production	'electricity production, wind, 1-3MW turbine, onshore - RoW - electricity, high voltage'	1
	Plant Construction	'wind turbine construction, 2MW, onshore - GLO - wind turbine, 2MW, onshore'	$1.18x10^{-8}$
	Raw Fuel Extraction	N/A	N/A
	Fuel Preparation	N/A	N/A
Wind (Offshore)	Energy Production	'electricity production, wind, 1-3MW turbine, offshore - RoW - electricity, high voltage'	1
	Plant Construction	'wind power plant construction, 2MW, offshore, moving parts - GLO - wind power plant, 2MW, offshore, moving parts'	$9.50x10^{-9}$
	Raw Fuel Extraction	N/A	N/A
	Fuel Preparation	N/A	N/A
Wind (Averaged)	Energy Production	N/A	N/A
	Plant Construction	N/A	N/A
	Raw Fuel Extraction	N/A	N/A
	Fuel Preparation	N/A	N/A
Solar	Energy Production	'electricity production, solar tower power plant, 20 MW - RoW - electricity, high voltage'	1
	Plant Construction	'concentrated solar power plant construction, solar tower power plant, 20 MW - RoW - concentrated solar power plant, solar tower, 20 MW'	$3.15x10^{-10}$
	Raw Fuel Extraction	N/A	N/A
	Fuel Preparation	N/A	N/A
Bioenergy	Energy Production	'heat and power co-generation, wood chips, 6667 kW - RoW - electricity, high voltage'	1
	Plant Construction	'heat and power co-generation unit construction, organic Rankine cycle, 1000kW electrical - GLO - heat and power co-generation unit, organic Rankine cycle, 1000kW electrical'	$8.28x10^{-9}$
	Raw Fuel Extraction	'market for slab and siding, softwood, wet, measured as dry mass - RoW - slab and siding, softwood, wet, measured as dry mass'	0.847
	Fuel Preparation	'wood chips production, softwood, at sawmill - RoW - wood chips, wet, measured as dry mass'	0.847
Other Renewables (Averaged)	Energy Production	N/A	N/A
	Plant Construction	N/A	N/A
	Raw Fuel Extraction	N/A	N/A
	Fuel Preparation	N/A	N/A

Table 6-25 – Objective LCA indicator results for the considered energy generation sources.

Impact Indicator	Unit	Energy Generation Objective Impacts										
		Coal	Gas	Oil	Nuclear	Hydro (Run-of-River)	Wind (1-3MW Onshore)	Wind (1-3MW Offshore)	Wind (Avg)	Solar	Bioenergy (Woodchips)	Other Renewable Electricity Excluding Bioenergy
Global Warming Potential (GWP 100)	kg CO_2-eq / kWh	1.12E+00	5.22E-01	1.14E+00	1.53E-02	8.57E-03	2.77E-02	2.34E-02	2.56E-02	5.90E-02	1.28E-01	3.11E-02
Ozone Depletion	kg CFC11-eq / kWh	4.90E-09	4.95E-08	6.23E-07	1.45E-09	5.43E-10	1.88E-09	1.00E-09	1.44E-09	4.21E-09	3.80E-08	2.06E-09
Metal Resource Depletion	kg Fe-eq / kWh	5.62E-03	5.05E-03	1.77E-02	1.25E-02	3.51E-03	2.06E-02	1.71E-02	1.88E-02	2.13E-02	1.13E-02	1.45E-02
Freshwater Eutrophication Potential	kg P-eq / kWh	9.31E-04	8.60E-06	3.52E-05	1.82E-03	2.11E-06	1.30E-05	9.52E-06	1.13E-05	1.26E-05	4.92E-05	8.67E-06
Marine Eutrophication Potential	kg N-eq / kWh	1.56E-03	1.56E-04	1.73E-03	1.56E-04	1.31E-05	3.69E-05	3.06E-05	3.37E-05	4.67E-05	1.19E-03	3.12E-05
Acidification Potential (Terrestrial)	kg SO2-eq / kWh	8.91E-03	4.28E-04	9.42E-03	1.05E-04	3.26E-05	1.35E-04	1.15E-04	1.25E-04	2.55E-04	1.98E-03	1.37E-04
Water Use	m3 / kWh	4.64E-03	1.61E-03	1.12E-03	3.20E-03	2.36E-05	1.14E-04	9.22E-05	1.03E-04	2.65E-04	2.59E-04	1.31E-04

Table 6-26 - Normalised LCA indicator results for the considered energy generation sources.

Impact Indicator	Unit	Normalised Energy Generation Impacts										
		Coal	Gas	Oil	Nuclear	Hydro (Run-of-River)	Wind (1-3MW Onshore)	Wind (1-3MW Offshore)	Wind (Avg)	Solar	Bioenergy (Woodchips)	Other Renewable Electricity Excluding Bioenergy
Global Warming Potential (GWP 100)	N.D.	9.79E-01	4.57E-01	1.00E+00	1.34E-02	7.51E-03	2.43E-02	2.05E-02	2.24E-02	5.18E-02	1.12E-01	2.72E-02
Ozone Depletion	N.D.	7.86E-03	7.94E-02	1.00E+00	2.32E-03	8.71E-04	3.02E-03	1.60E-03	2.31E-03	6.76E-03	6.11E-02	3.31E-03
Metal Resource Depletion	N.D.	2.64E-01	2.38E-01	8.31E-01	5.89E-01	1.65E-01	9.70E-01	8.03E-01	8.87E-01	1.00E+00	5.32E-01	6.84E-01
Freshwater Eutrophication Potential	N.D.	5.11E-01	4.72E-03	1.93E-02	1.00E+00	1.16E-03	7.15E-03	5.22E-03	6.19E-03	6.92E-03	2.70E-02	4.76E-03
Marine Eutrophication Potential	N.D.	9.05E-01	9.05E-02	1.00E+00	9.02E-02	7.59E-03	2.13E-02	1.77E-02	1.95E-02	2.70E-02	6.88E-01	1.80E-02
Acidification Potential (Terrestrial)	N.D.	9.47E-01	4.54E-02	1.00E+00	1.12E-02	3.46E-03	1.43E-02	1.22E-02	1.33E-02	2.71E-02	2.11E-01	1.46E-02
Water Use	N.D.	1.00E+00	3.47E-01	2.42E-01	6.90E-01	5.08E-03	2.45E-02	1.99E-02	2.22E-02	5.71E-02	5.58E-02	2.81E-02

With impact indicator values quantified for each of the generation sources via a uniform methodology, they can be fairly compared. To facilitate this, the data is normalised across each indicator, using Equation 6-4 to determine the relative impacts of each technology ($\hat{I}_{n_j}$), This results in the values shown in Table 6-26, where higher values indicate more severe impacts.

Equation 6-4 – Normalisation procedure used for energy generation impacts. where I_{n_j} is nth indicator score for generation source j, and $I_{n_{Max}}$ is the highest observed impact value for the nth indicator across all generation sources.

$$\hat{I}_{n_j} = \frac{I_{n_j}}{I_{n_{Max}}}$$

Figure 6-18 graphically displays this normalised data on a logarithmic axis, necessitated due to the elevated impacts observed for fossil routes. It is clearly seen that coal and oil are the worst-performing options. Interestingly, all generation sources exhibit similarly poor performance within the mineral resource depletion indicator (average normalised value of 0.633); this is attributable to the heavy use of abiotic resources in the production of PV cells and wind turbines, with causation appearing less obvious for hydro and bioenergy. The evaluated alternatives exhibit relatively concentric impact profiles, revealing hydro as the best performing alternative within all assessed indicators. This is thought to be a consequence of the relatively basic construction of run-of-river plants and their lack of feedstock requirements and operational emissions.

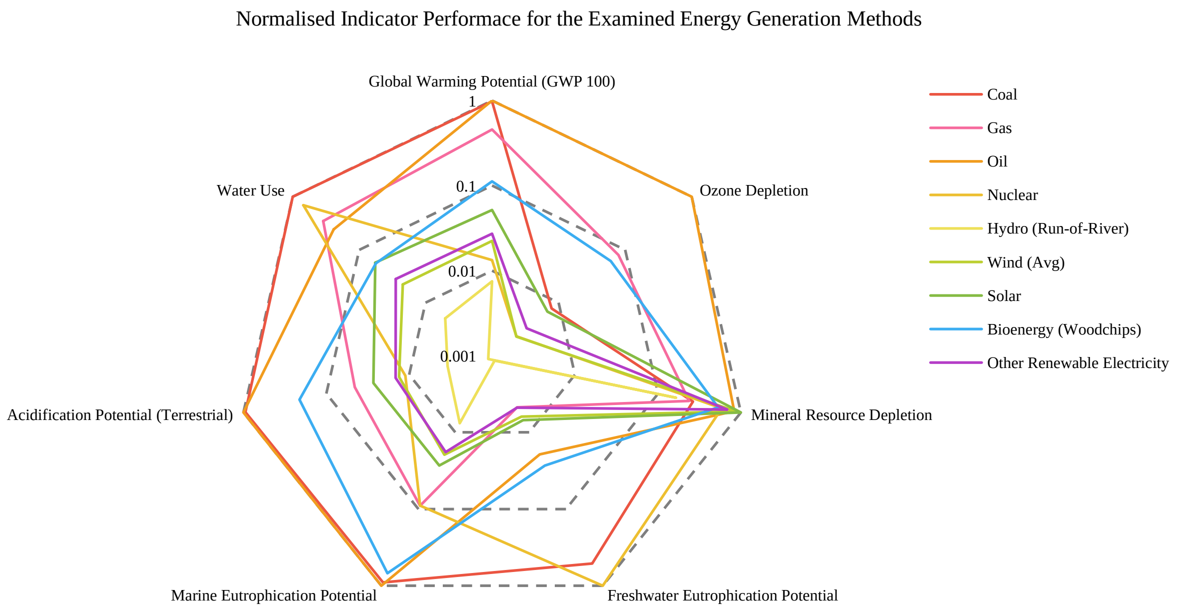


Figure 6-18 – LCA indicator performance of assessed energy generation sources. Where higher values show higher impact potential.

These alternative generation routes can be further examined by averaging their normalised impact indicator values to obtain an overall score via Equation 6-5, resulting in Figure 6-19. The data confirms that hydroelectric is the most sustainable energy generation source with respect to the selected environmental indicators. Coal and oil are significantly worse performing than all other options, aligning with the expected results; in fact, oil receives an average normalised score of one, confirming that it has the highest impact burden across all categories. Additionally, gas exhibits a surprisingly low average normalised impact score, performing marginally better than bioenergy.

Equation 6-5 – Calculation of the average normalised performance across the seven impact indicators for each generation source.

$$\bar{\bar{I}}_j = \frac{\sum_{i=1}^{n}(\hat{I}_{j_i})}{7}$$

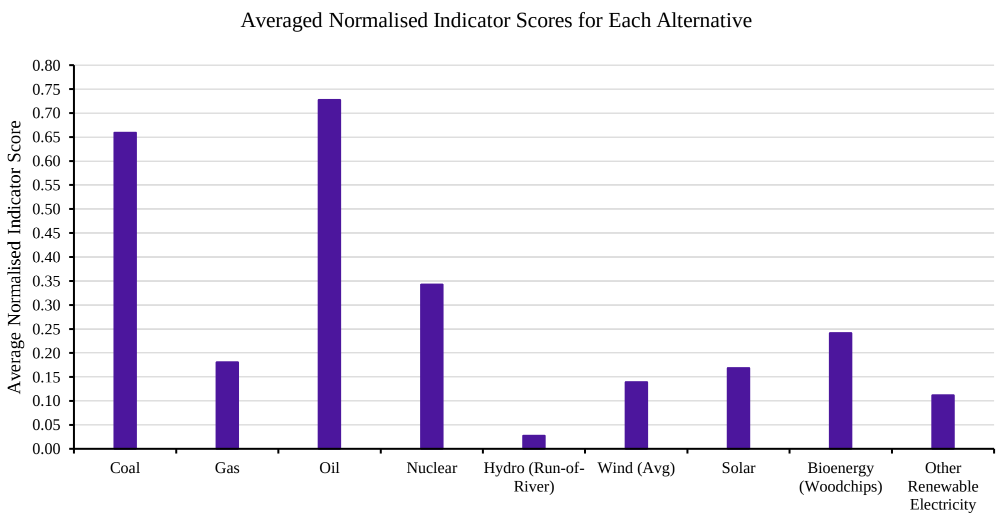


Figure 6-19 – Average of the normalised impact indicator values for each considered energy generation source.

6.6.3.2 Grid Mix Impact Calculation

With impacts characterised for all generation sources on a 1 kWh basis, national grid mix composition data can be utilised to examine the environmental impacts of electricity supplies within specific countries using Equation 6-6. This enables the proof-of-concept study to evaluate representative electricity impact profiles for all 206 countries covered by the grid composition data from literature [293]. Again, only the G20 is presented in the body of this thesis, evaluating their grid electricity impacts via Equation 6-6.

Equation 6-6 – Calculation of overall national grid impact indicator values per kWh. Where, $GS_{n,i}$ is the percentage grid share of generation source i in country n, and I_{y_i} is the impact indicator y value of generation source i per kWh.

$$Country\ n\ indicator\ y\ value = \sum_{i=1}^{9}\left(\left(\frac{GS_{n,i}}{100}\right) \times I_{y_i}\right)$$

Figure 6-20 shows that the G20 countries' electricity impact profiles over the proof-of-concept's selected indicators are relatively similar. However, due to the proximity of many of the results, the figure is somewhat difficult to interpret. To overcome this, the impacts are also evaluated in terms of the mean absolute difference (MAD), and relative mean absolute difference (RMAD) using Equation 6-7 and Equation 6-8, the degree of variation can be independently quantified for each indicator. Large MAD values indicate a greater spread of observed values, and small MAD values indicate broadly similar results.

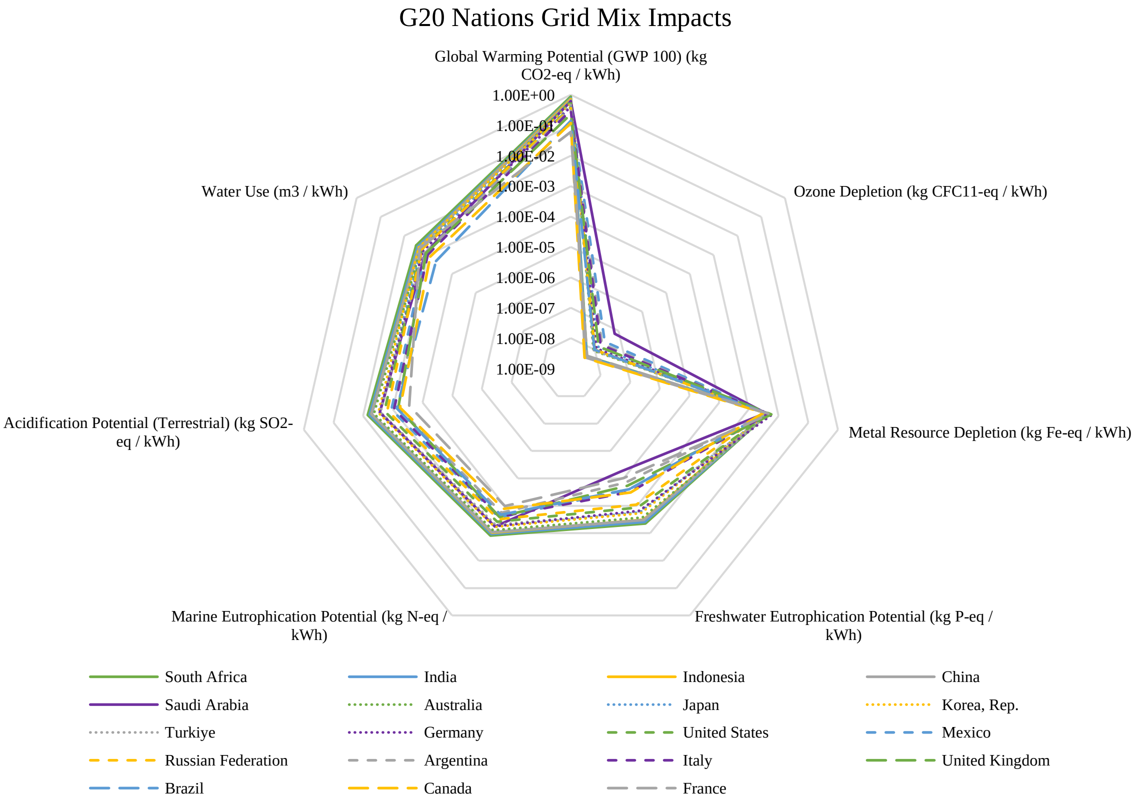


Figure 6-20 – Objective indicator results for the grid mixes of G20 countries (excluding the EU) on a logarithmic scale.

Equation 6-7 – Calculation procedure for the mean absolute difference observed in each indicator across the G20 nation's electricity grids. Where, n is the number of countries examined, x_i are the data values in the set, and $m(X)$ is the mean value of the set.

$$MAD = \frac{1}{n}\sum_{i=i}^{n}|x_i - m(X)|$$

Equation 6-8 – Calculation of the relative mean absolute difference (RMAD) observed in each indicator across the G20 nation's electricity grids. Where MAD is the mean absolute difference and $m(X)$ is the mean value of the set.

$$RMAD = \frac{MAD}{m(X)}$$

Consideration of the RMAD adds value to the analysis as it removes the influence of the indicator values' magnitude which is present in the original MAD value. A pertinent example of this is the ozone depletion indicator. With the lowest average indicator value across the G20 (excluding the EU), at 4.405E-08 kg CFC11-ep / kWh, the MAD appears to be insignificant (3.219E-08); however, once adjusted to account for the low average magnitude, the RMAD reveals significant differences in national grid impacts (supported visually by Figure 6-20).

Table 6-27 – Mean absolute difference (MAD) and relative mean absolute difference observed in the G20's objective grid impacts relative to each indicator. MAD and RMAD results for each indicator have been colour coded to represent the magnitude of the observed differences, where green shows low difference and red shows high difference.

Indicator	Global Warming Potential	Ozone Depletion	Metal Resource Depletion	Freshwater Eutrophication Potential	Marine Eutrophication Potential	Acidification Potential (Terrestrial)	Water Use
Mean Absolute Difference (MAD)	1.982E-01	3.219E-08	1.262E-03	2.524E-04	3.015E-04	1.809E-03	7.755E-04
Relative Mean Absolute Difference (RMAD)	7.276E+00	1.388E+01	2.907E+00	1.037E+01	9.331E+00	1.111E+01	6.793E+00

Each of the G20 countries' grid mix impact indicator values are shown in Table 6-28 for transparency. It is recognised that the quantity of data makes interpretation a challenge; therefore, the impacts realised by each country are colour coded on an indicator-by-indicator basis. An interesting result is observed in the poor eutrophication potential performance of the French electricity grid. However, by consulting the data in Table 6-20 and Table 6-25 this can be explained by the high utilisation of nuclear energy (~68%), and the generation sources high contribution to eutrophication (highest observed across all alternatives). South Africa is seen to exhibit poor GWP performance. Again, the literature data and LCIA results for the generation sources reveal the causal factor, in this case heavy reliance on coal plants (~86%), the second worst alternative after oil with respect to GWP. Generally, very positive performance is seen across the full suite of indicators form the Brazilian grid, a result of high hydro utilisation (~55%) and its position as the best performing alternative overall (ref. Figure 6-19). Of the G20 nations, South Africa realises the highest electricity grid impacts, with Canada achieving the lowest impact per kWh, reflecting the countries portfolio of renewable generation sources and adoption of gas over dirtier coal or oil alternative for a majority of the remaining fossil generation.

Table 6-28 – Objective numerical impact indicator results for the G20's (excluding the EU) national electricity grid (quantified per kWh).

Country	Global Warming Potential (GWP 100) (kg CO_2-eq / kWh)	Ozone Depletion (kg CFC11-eq / kWh)	Metal Resource Depletion (kg Fe-eq / kWh)	Freshwater Eutrophication Potential (kg P-eq / kWh)	Marine Eutrophication Potential (kg N-eq / kWh)	Acidification Potential (Terrestrial) (kg SO2-eq / kWh)	Water Use (m3 / kWh)
Argentina	4.036E-01	6.311E-08	7.549E-03	1.532E-04	2.461E-04	9.674E-04	1.366E-03
Australia	6.974E-01	2.340E-08	8.845E-03	4.832E-04	8.852E-04	4.884E-03	2.735E-03
Brazil	1.741E-01	3.247E-08	7.276E-03	8.523E-05	2.596E-04	9.368E-04	5.616E-04
Canada	1.421E-01	9.976E-09	6.256E-03	3.129E-04	1.671E-04	6.880E-04	9.375E-04
China	7.300E-01	6.759E-09	7.364E-03	6.763E-04	1.029E-03	5.705E-03	3.156E-03
France	8.020E-02	1.615E-08	1.177E-02	1.269E-03	1.890E-04	4.091E-04	2.394E-03
Germany	4.665E-01	3.665E-08	1.112E-02	4.902E-04	6.581E-04	3.163E-03	2.065E-03
India	8.566E-01	7.425E-09	6.858E-03	7.397E-04	1.201E-03	6.701E-03	3.610E-03
Indonesia	8.141E-01	2.744E-08	6.367E-03	5.769E-04	1.086E-03	5.859E-03	3.191E-03
Italy	3.825E-01	5.443E-08	8.403E-03	5.709E-05	3.161E-04	1.218E-03	1.140E-03
Japan	5.971E-01	4.200E-08	7.910E-03	4.266E-04	6.831E-04	3.476E-03	2.356E-03
Korea, Rep.	5.773E-01	2.535E-08	8.207E-03	8.034E-04	6.979E-04	3.511E-03	2.989E-03
Mexico	4.701E-01	9.013E-08	8.161E-03	1.095E-04	3.541E-04	1.571E-03	1.380E-03
Russian Federation	4.254E-01	2.651E-08	6.527E-03	5.305E-04	3.831E-04	1.818E-03	2.136E-03
Saudi Arabia	7.633E-01	2.743E-07	1.004E-02	1.904E-05	7.725E-04	3.952E-03	1.417E-03
South Africa	9.754E-01	8.577E-09	7.027E-03	9.041E-04	1.375E-03	7.778E-03	4.203E-03
Turkiye	5.312E-01	2.307E-08	7.450E-03	2.900E-04	5.708E-04	2.988E-03	1.994E-03
United Kingdom	2.899E-01	4.296E-08	1.090E-02	3.097E-04	3.257E-04	9.129E-04	1.325E-03
United States	4.593E-01	2.626E-08	8.612E-03	5.492E-04	4.628E-04	2.239E-03	2.253E-03

It is hoped that this example of environmental LCI generation for the model outlines the general depth and steps taken across all considered spoke sets within the proof-of-concept study. For each set the application of system boundaries is kept consistent and systematic across all competing alternatives, employing the same databases and characterisation methods.

For the TEA assessment strand, economic data is collected for national electricity grid wholesale prices before any relevant temporal adjustments for inflation are applied [290], and local currency is converted to GBP using the average 2022 exchange rates [291]. The social indicators are assessed based on country of deployment using the characterisation methods developed in Chapter 5.

6.6.4 Spoke Data Sets

Using the previously detailed approach to LCI generation, the remaining Hou process inputs (spoke sets) are evaluated. The data sheets for each assessed spoke are provided in Appendix C. Within these the temporal and geographic setting, system boundary diagram, and process description are given, providing an overview of the data quality and LCI coverage. Applying analogous methodologies to those presented in Section 6.6.3.1, the objective impacts of each spoke across the 19 selected indicators are detailed in full within Table 6-29. Normalised values, calculated at the spoke set level, are also given in Table 6-30. Examination of the resulting data and its associated insight generation is approached in the following section.

6.7 Results & Discussion

In the results and discussion section of this chapter, the MCDM performance is evaluated and compared to the theoretical workload savings predicted in Chapter 4. Individual spoke's impact results are then detailed and discussed, before examining relative performance within each of the sets. Identification of well performing value chains is then approached via AHP-TOPSIS derived local rankings (Section 4.5.2.4) and the aggregation procedure laid out in Sections 4.5.3.6 and 4.5.3.7. These results are then examined in the context of framework efficacy and behaviour within the discussion. Following this consideration of the 'unweighted' value chain recommendations, the effects of MCDM inputs on spoke selection and value chain recommendations are examined for rank reversal. Confirmation that the decision maker value choice inputs exercise appropriate control over the value chain recommendations is a necessary part of the framework validation, allowing FMCG companies to tailor strategic and sustainable development to their needs and priorities. Throughout, the efficacy, strengths, and weaknesses of the developed methodology are discussed.

6.7.1 MCDM Performance

As detailed in Section 4.5.2 of Chapter 4, the tiered AHP structure is selected as a method for reducing practitioner workloads relative to the more traditional global approach (Figure 4-8). It was determined that a maximum reduction of the required pairwise comparisons (68.63%) was attained for assessments with a total of 18 indicators, distributed evenly across the three assessment strands [203]. This is not the scenario realised within the proof-of-concept, instead evaluating 19 indicators with a non-uniform distribution.

Using Equation 4-1 the number of pairwise comparisons required within the proof-of-concept study is 171 using a global AHP structure; a prohibitive workload in real life applications. However, considering the tiered structure with a 7-5-7 distribution of indicators by strand (LCA, TEA, SIA respectively), only 55 pairwise comparisons are required. This represents a 67.84% reduction, achieving close to optimal efficiency for practitioners in a real application. While the distribution of indicators within strands is relatively close to uniform, this confirms the effectiveness of a tiered structure over the global alternative.

Compounding this, as the number of pairwise comparisons within a single AHP matrix increases, acceptable consistency ratios become harder to achieve. Therefore, practitioners or decision makers using a global approach would have to make multiple passes, correcting inconsistencies in their prescriptions. The tiered structure is effective in combatting this as it partitions pairwise comparisons into sub-matrices. A general solution to the percentage workload saving in assessments with evenly distributed indicators is given by Equation 6-9. When plotted into high indicator counts, it is revealed that the workload reduction achieved stabilises around a value of 66.78%, showing that the techniques effectiveness diminishes little with increasing indicator count (Figure 6-21).

Equation 6-9 – General solution for the workload reduction achieved by the adoption of tiered AHP (assuming even indicator distribution between strands). Where, S is the number of assessment strands and C is the total indicator count.

$$Workload\ Saving\ (\%) = \frac{\left(\left(\frac{(C^2 - C)}{2}\right) - \left(S\left(\frac{\left(\frac{C}{S}\right)^2 - \left(\frac{C}{S}\right)}{2}\right) + \frac{S^2 - S}{2}\right)\right)}{\left(S\left(\frac{\left(\frac{C}{S}\right)^2 - \left(\frac{C}{S}\right)}{2}\right) + \frac{S^2 - S}{2}\right)} \times 100$$

Utilising Equation 6-9, the performance of tiered AHP can be evaluated for alternate assessment configurations. Double stranded assessments (typically integrated LCA-TEAs [19] [39]) are becoming increasingly common within literature. If the hub and spoke framework were utilised in such an assessment, the tiered AHP approach would also offer significant, but lesser, workload savings; peaking at a 53.57% reduction in pairwise comparisons as shown by Figure 6-21 (for 8 indicators). While providing less benefit than the initially targeted triple stranded assessments, the data demonstrates broad utility of the developed framework.

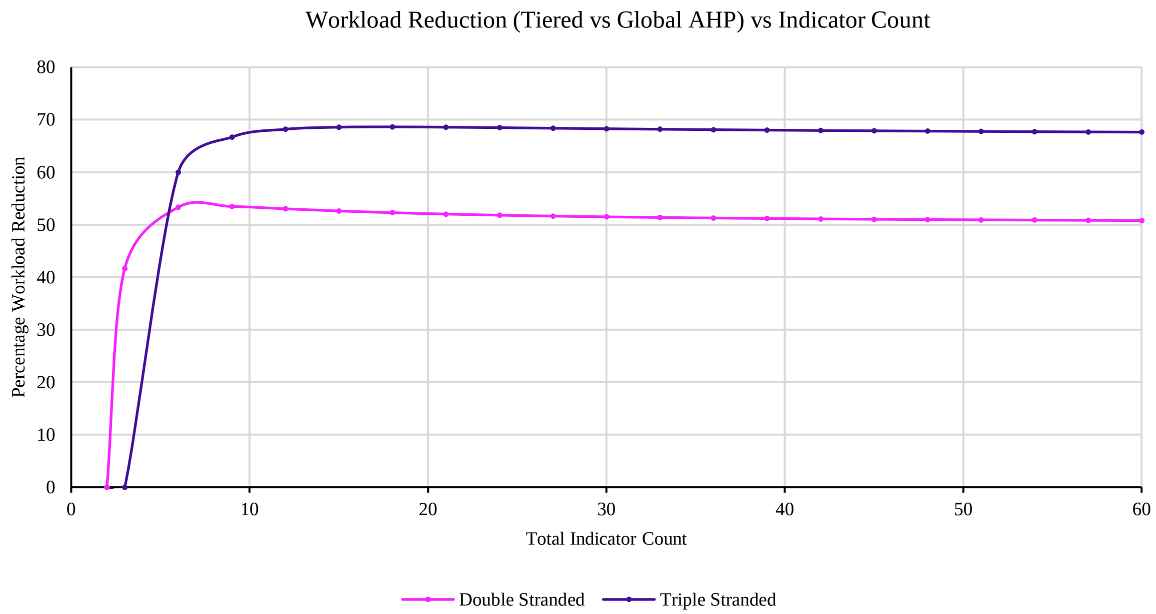


Figure 6-21 - Percentage workload savings for tiered AHP in double and triple stranded assessment configurations as total indicator count increases.

6.7.2 Spoke Set's Local Indicator Results

For each of the spoke sets evaluated (ammonia, sodium chloride, carbon dioxide, electricity and heat) objective impact indicator results are calculated based on the mass balances and systems boundaries specified in the corresponding data sheets (Appendix C). This impact quantification deploys the characterisation methods selected in Section 6.5.2.1 and delivers the results shown in Table 6-29. The impacts are reported relative to the local functional unit; per tonne produced for materials, or per kWh for energy. The use of different functional units between spoke sets clearly prevents any equitable comparisons. Consequently, the values for each indicator are normalised within each of the spoke sets using the procedures specified in Section 4.5.3.4 (specifically Equation 4-7 and Equation 4-8), allowing the comparison of relative performance against a uniform scale. Due to the homologation of scoring directionality, specified within the framework's methodology, all indicators report high scores for a favourable normalised result (maximum of 1, minimum of 0). The results of this intra-set normalisation allow for easier comparison of the available alternatives. Figure 6-22 to Figure 6-26 reflect the indicator performance profiles of spoke sets 1 to 5 respectively.

Figure 6-22, examining the ammonia feedstock production routes, shows a stronger performance from China than India across the SIA indicators, suggesting lower risk of negative impacts across all nine examined areas. Furthermore, China is only beaten by Germany (included for comparison to a hypothetical European alternative) in four of the nine indicators. When examining the LCA indicators, country of operation has less influence. Rather, predictively, the alternatives indicator values diverge based on technological route. Biogas fed steam methane reformation (SMR) Haber-Bosch (HB) offers the best performance in all LCA indicators irrespective of location. The routes combining wind-based proton exchange membrane (PEM) and eHB (both India and China) perform similarly apart from their poor performance in metal resource depletion; a consequence of their reliance on titanium, gold, iridium and platinum for electrodes and other components [300]. In a surprising result, the natural gas fed SMR HB route performs much better than the grid powered PEM and HB option. With the traditional SMR HB route's 1.22 t_{CO_2}/t_{NH_3} [301] stoichiometric emissions, this speaks to the severity of both Indian and Chinese grid electricity generation impacts, heavily penalising the significant energy demand of PEM hydrogen production ($3.82 \times 10^4\ kWh/t_{NH_3}$). In the case of China and India, significant proportions of the grid mixes still rely on fossil fuels (66.3 and 78.1% respectively). OpEx was relatively consistent across all routes (SMR HB (China) performing best), exhibiting a range of 517-617 GBP/tonne.

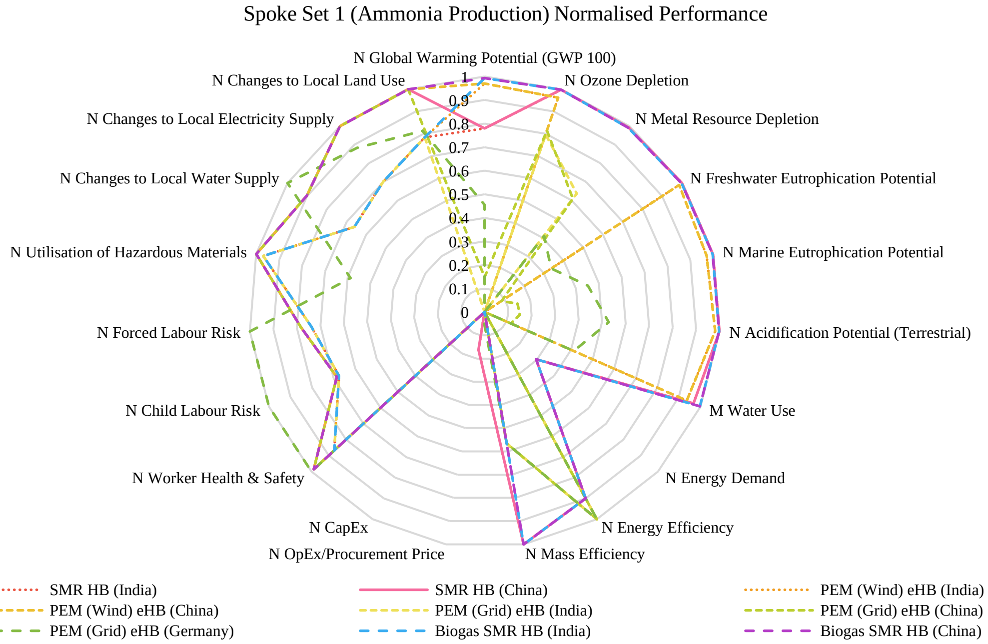


Figure 6-22 – Relative performance of spokes within set 1 against the proof-of concept indicators (normalised).

Figure 6-23 shows the performance of the assessed sodium chloride production routes. Rock salt mining can be visually identified as a clear best route, significantly reducing impacts within all environmental indicators. With the natural deposits being mined directly from high purity deposits, the only remaining processing step is pulverisation or crushing (dependent on use). Consequently, it's strong relative environmental performance is of little surprise when considering the additional energy intensive processing steps such as evaporation within solution mining. The rock salt mining options diverge when examining the social indicators, revealing China as the preferable option in all cases. In addition, the rock salt routes perform best in all but one (OpEx, in which solution mining is the best performing alternative) of the economic indicators. It is therefore expected that the aggregation procedure employed within the framework will favour rock salt mining in China (spoke ID 2.6) when recommending optimal value chain structures.

Perhaps unsurprisingly, the performance of solution mining routes is very poor in the water usage indicator, owing to the pumping of water into sub-terranean deposits for dissolution and subsequent evaporation to obtain solid NaCl. The large quantities of water utilised are typically then lost to evaporation with no condensation apparatus employed to achieve a circular solvent loop [302]. Indirect and direct methods primarily differ in the salts extracted from the natural deposits. Direct solution mining extracts dissolved sodium chloride while indirect methods extract magnesium and calcium chlorides; these are subsequently converted to sodium chloride through the addition of sodium sulphate (mined from natural mineral deposits). Precipitated calcium carbonate is also obtained as a potentially saleable by-product through the indirect route. However, given the additional impact burden associated with the extra processing steps and feedstocks, the route is overall less competitive than the direct alternative.

Table 6-29 – Objective indicator results for the assessed spoke systems.

Indexing		Objective Results																		
Spoke	ID	Global Warming Potential (GWP 100) (kg CO_2-eq / FU)	Ozone Depletion (kg CFC-11-eq. / FU)	Metal Resource Depletion (kg Cu-eq. / FU)	Freshwater Eutrophication Potential (kg P-eq. / FU)	Marine Eutrophication Potential (kg N-eq. / FU)	Acidification Potential (Terrestrial) (kg SO_2-eq. / FU)	Water Use (m^3 / FU)	Energy Demand (MJ / FU)	Energy Efficiency (%)	Mass Efficiency (%)	OpEx/Procurement Price (2022 GBP / FU)	CapEx (2022 GBP / FU)	Worker Health & Safety (N.D.)	Child Labour Risk (N.D.)	Forced Labour Risk (N.D.)	Utilisation of Hazardous Materials (N.D.)	Changes to Local Water Supply (N.D.)	Changes to Local Electricity Supply (N.D.)	Changes to Local Land Use (N.D.)
SMR HB (India)	1.1	2.00E+03	1.00E-06	1.37E+00	3.32E-03	1.36E-02	4.02E-02	1.30E+00	2.69E+04	9.00E+01	9.82E+01	5.17E+02	0.00E+00	6.12E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
SMR HB (China)	1.2	2.00E+03	1.00E-06	1.37E+00	3.32E-03	1.36E-02	4.02E-02	1.30E+00	2.69E+04	9.00E+01	9.82E+01	5.17E+02	0.00E+00	6.94E-01	6.17E-01	7.34E-01	4.92E-01	6.80E-01	2.78E-01	7.55E-01
PEM (Wind) eHB (India)	1.3	2.71E+02	1.50E-05	2.00E+02	1.20E-01	3.58E-01	1.32E+00	2.52E+00	3.82E+04	1.00E+02	5.55E+01	6.17E+02	0.00E+00	6.12E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
PEM (Wind) eHB (China)	1.4	2.71E+02	1.50E-05	2.00E+02	1.20E-01	3.58E-01	1.32E+00	2.52E+00	3.82E+04	1.00E+02	5.55E+01	6.17E+02	0.00E+00	6.94E-01	6.17E-01	7.34E-01	4.92E-01	6.80E-01	2.78E-01	7.55E-01
PEM (Grid) eHB (India)	1.5	9.09E+03	7.90E-05	7.28E+01	7.85E+00	1.27E+01	7.11E+01	3.97E+01	3.82E+04	1.00E+02	5.55E+01	6.17E+02	0.00E+00	6.12E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
PEM (Grid) eHB (China)	1.6	7.75E+03	7.20E-05	7.81E+01	7.18E+00	1.09E+01	6.05E+01	3.49E+01	3.82E+04	1.00E+02	5.55E+01	6.17E+02	0.00E+00	6.94E-01	6.17E-01	7.34E-01	4.92E-01	6.80E-01	2.78E-01	7.55E-01
PEM (Grid) eHB (Germany)	1.7	4.95E+03	3.89E-04	1.18E+02	5.20E+00	6.98E+00	3.36E+01	2.33E+01	3.82E+04	1.00E+02	5.55E+01	5.98E+02	0.00E+00	7.05E-01	9.00E-01	9.38E-01	2.89E-01	7.53E-01	2.45E-01	6.14E-01
Biogas SMR HB (India)	1.8	6.34E+01	1.00E-06	1.78E+00	1.38E-02	2.72E-02	1.38E-01	1.10E-01	2.69E+04	9.00E+01	9.82E+01	6.17E+02	0.00E+00	6.12E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
Biogas SMR HB (China)	1.9	6.34E+01	1.00E-06	1.78E+00	1.38E-02	2.72E-02	1.38E-01	1.10E-01	2.69E+04	9.00E+01	9.82E+01	6.17E+02	0.00E+00	6.94E-01	6.17E-01	7.34E-01	4.92E-01	6.80E-01	2.78E-01	7.55E-01
Direct Solution Mining (India)	2.1	1.75E+03	1.01E-04	3.83E+02	1.14E+00	1.30E+00	7.04E+00	1.11E+01	1.35E+04	9.18E+01	1.00E+02	7.03E+01	0.00E+00	6.12E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
Direct Solution Mining (China)	2.2	1.75E+03	1.01E-04	3.83E+02	1.14E+00	1.30E+00	7.04E+00	1.11E+01	1.35E+04	9.18E+01	1.00E+02	2.04E+02	0.00E+00	6.94E-01	6.17E-01	7.34E-01	4.92E-01	6.80E-01	2.78E-01	7.55E-01
Indirect Solution Mining (India)	2.3	2.77E+03	1.56E-04	1.50E+02	4.60E-01	1.45E+00	8.21E+00	1.13E+01	2.06E+04	9.18E+01	9.88E+01	3.66E+02	0.00E+00	6.12E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
Indirect Solution Mining (China)	2.4	2.77E+03	1.56E-04	1.50E+02	4.60E-01	1.45E+00	8.21E+00	1.13E+01	2.06E+04	9.18E+01	9.88E+01	5.34E+02	0.00E+00	6.94E-01	6.17E-01	7.34E-01	4.92E-01	6.80E-01	2.78E-01	7.55E-01
Rock Salt Mining (India)	2.5	2.55E+02	8.00E-06	5.39E+01	1.54E-01	3.82E-01	1.45E+00	3.97E+00	2.01E+02	1.00E+02	1.00E+02	2.29E+02	0.00E+00	6.12E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
Rock Salt Mining (China)	2.6	2.55E+02	8.00E-06	5.39E+01	1.54E-01	3.82E-01	1.45E+00	3.97E+00	2.01E+02	1.00E+02	1.00E+02	2.29E+02	0.00E+00	6.94E-01	6.17E-01	7.34E-01	4.92E-01	6.80E-01	2.78E-01	7.55E-01
DAC (India)	3.1	-1.51E+02	1.00E-06	1.19E+00	8.28E-02	1.37E-01	7.52E-01	1.80E+00	6.93E+03	9.06E+01	1.00E+02	8.12E+02	0.00E+00	6.12E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
DAC (China)	3.2	-1.64E+02	1.00E-06	1.24E+00	7.58E-02	1.18E-01	6.42E-01	1.75E+00	6.93E+03	9.06E+01	1.00E+02	8.12E+02	0.00E+00	6.94E-01	6.17E-01	7.34E-01	4.92E-01	6.80E-01	2.78E-01	7.55E-01
DAC (Germany)	3.3	-1.93E+02	4.00E-06	1.66E+00	5.53E-02	7.71E-02	3.63E-01	1.63E+00	6.93E+03	9.06E+01	1.00E+02	8.12E+02	0.00E+00	7.05E-01	9.00E-01	9.38E-01	2.89E-01	7.53E-01	2.45E-01	6.14E-01
MEA (India)	3.4	-1.86E+02	2.30E-05	5.68E+01	2.14E-01	6.24E-01	2.31E+00	3.74E+00	3.38E+03	9.00E+01	9.95E+01	3.53E+01	0.00E+00	6.12E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
MEA (China)	3.5	-1.86E+02	2.30E-05	5.68E+01	2.14E-01	6.24E-01	2.31E+00	3.74E+00	3.38E+03	9.00E+01	9.95E+01	3.53E+01	0.00E+00	6.94E-01	6.17E-01	7.34E-01	4.92E-01	6.80E-01	2.78E-01	7.55E-01

Indexing		Objective Results																			
Spoke	ID	Global Warming Potential (GWP 100) (kg CO_2-eq / FU)	Ozone Depletion (kg CFC-11-eq. / FU)	Metal Resource Depletion (kg Cu-eq. / FU)	Freshwater Eutrophication Potential (kg P-eq. / FU)	Marine Eutrophication Potential (kg N-eq. / FU)	Acidification Potential (Terrestrial) (kg SO_2-eq. / FU)	Water Use (m^3 / FU)	Energy Demand (MJ / FU)	Energy Efficiency (%)	Mass Efficiency (%)	OpEx/Procurement Price (2022 GBP / FU)	CapEx (2022 GBP / FU)	Worker Health & Safety (N.D.)	Child Labour Risk (N.D.)	Forced Labour Risk (N.D.)	Utilisation of Hazardous Materials (N.D.)	Changes to Local Water Supply (N.D.)	Changes to Local Electricity Supply (N.D.)	Changes to Local Land Use (N.D.)
Wind (India)	4.1	2.56E-02	1.44E-09	1.88E-02	1.13E-05	3.37E-05	1.25E-04	1.03E-04	0.00E+00	1.00E+02	1.00E+02	4.06E-02	0.00E+00	3.88E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
Solar (India)	4.2	5.90E-02	4.21E-09	2.13E-02	1.26E-05	4.67E-05	2.55E-04	2.65E-04	0.00E+00	1.00E+02	1.00E+02	4.06E-02	0.00E+00	3.88E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
Bioenergy (India)	4.3	1.28E-01	3.80E-08	1.13E-02	4.92E-05	1.19E-03	1.98E-03	2.59E-04	0.00E+00	1.00E+02	1.00E+02	4.87E-02	0.00E+00	3.88E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
Hydro (India)	4.4	8.57E-03	5.43E-10	3.51E-03	2.11E-06	1.31E-05	3.26E-05	2.36E-05	0.00E+00	1.00E+02	1.00E+02	4.87E-02	0.00E+00	3.88E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
CHP, Lignite (India)	4.5	1.31E+00	3.45E-09	3.72E-03	2.50E-03	1.47E-03	7.06E-03	6.32E-03	0.00E+00	1.00E+02	1.00E+02	3.79E-02	0.00E+00	3.88E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
CHP, Oil (India)	4.6	8.58E-01	8.89E-08	4.39E-03	1.67E-05	1.12E-03	6.50E-03	7.21E-04	0.00E+00	1.00E+02	1.00E+02	3.79E-02	0.00E+00	3.88E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
CHP, Biogas (India)	4.7	2.09E-01	3.89E-09	6.62E-03	4.12E-05	1.49E-04	1.51E-03	2.27E-04	0.00E+00	1.00E+02	1.00E+02	4.87E-02	0.00E+00	3.88E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
CHP, Natural Gas (India)	4.8	6.38E-01	3.44E-08	1.13E-02	1.20E-05	2.68E-04	7.29E-04	2.57E-03	0.00E+00	1.00E+02	1.00E+02	3.33E-02	0.00E+00	3.88E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
Grid (India)	4.9	8.57E-01	7.43E-09	6.86E-03	7.40E-04	1.20E-03	6.70E-03	3.61E-03	0.00E+00	1.00E+02	1.00E+02	1.05E-01	0.00E+00	3.88E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
CHP, Lignite (India)	5.1	6.68E-02	1.76E-10	1.91E-04	1.28E-04	7.50E-05	3.61E-04	3.23E-04	0.00E+00	1.00E+02	1.00E+02	3.79E-02	0.00E+00	3.88E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
CHP, Oil (India)	5.2	4.39E-02	4.55E-09	2.25E-04	8.57E-07	5.75E-05	3.32E-04	3.69E-05	0.00E+00	1.00E+02	1.00E+02	3.79E-02	0.00E+00	3.88E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
CHP, Biogas (India)	5.3	9.84E-03	1.84E-10	3.12E-04	1.94E-06	7.04E-06	7.13E-05	1.07E-05	0.00E+00	1.00E+02	1.00E+02	4.87E-02	0.00E+00	3.88E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
CHP, Natural Gas (India)	5.4	3.26E-02	1.76E-09	5.79E-04	6.13E-07	1.37E-05	3.73E-05	1.32E-04	0.00E+00	1.00E+02	1.00E+02	3.33E-02	0.00E+00	3.88E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
Natural Gas, Furnace (India)	5.5	6.90E-02	5.77E-09	3.61E-04	9.44E-07	1.59E-05	6.14E-05	1.24E-05	0.00E+00	1.00E+02	1.00E+02	5.12E-02	0.00E+00	3.88E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01
Biomass, Furnace (India)	5.6	1.71E-02	8.42E-10	1.13E-03	7.53E-06	5.31E-05	1.23E-04	5.97E-05	0.00E+00	1.00E+02	1.00E+02	7.49E-02	0.00E+00	3.88E-01	6.07E-01	6.93E-01	4.77E-01	4.98E-01	1.95E-01	5.91E-01

Table 6-30 – Normalised objective indicator results for the assessed spoke systems.

Indexing		Normalised Objective Results																		
Spoke	ID	Global Warming Potential (GWP 100)	Ozone Depletion	Metal Resource Depletion	Freshwater Eutrophication Potential	Marine Eutrophication Potential	Acidification Potential (Terrestrial)	Water Use	Energy Demand	Energy Efficiency	Mass Efficiency	OpEx/Procurement Price	CapEx	Worker Health & Safety	Child Labour Risk	Forced Labour Risk	Utilisation of Hazardous Materials	Changes to Local Water Supply	Changes to Local Electricity Supply	Changes to Local Land Use
SMR HB (India)	1.1	7.80E-01	9.97E-01	9.93E-01	1.00E+00	9.99E-01	9.99E-01	9.67E-01	2.96E-01	9.00E-01	1.00E+00	1.62E-01	0.00E+00	8.68E-01	6.75E-01	7.39E-01	9.70E-01	6.61E-01	7.01E-01	7.83E-01
SMR HB (China)	1.2	7.80E-01	9.97E-01	9.93E-01	1.00E+00	9.99E-01	9.99E-01	9.67E-01	2.96E-01	9.00E-01	1.00E+00	1.62E-01	0.00E+00	9.85E-01	6.86E-01	7.82E-01	1.00E+00	9.03E-01	1.00E+00	1.00E+00
PEM (Wind) eHB (India)	1.3	9.70E-01	9.61E-01	0.00E+00	9.85E-01	9.72E-01	9.81E-01	9.37E-01	0.00E+00	1.00E+00	5.65E-01	0.00E+00	0.00E+00	8.68E-01	6.75E-01	7.39E-01	9.70E-01	6.61E-01	7.01E-01	7.83E-01
PEM (Wind) eHB (China)	1.4	9.70E-01	9.61E-01	0.00E+00	9.85E-01	9.72E-01	9.81E-01	9.37E-01	0.00E+00	1.00E+00	5.65E-01	0.00E+00	0.00E+00	9.85E-01	6.86E-01	7.82E-01	1.00E+00	9.03E-01	1.00E+00	1.00E+00
PEM (Grid) eHB (India)	1.5	0.00E+00	7.97E-01	6.36E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	5.65E-01	0.00E+00	0.00E+00	8.68E-01	6.75E-01	7.39E-01	9.70E-01	6.61E-01	7.01E-01	7.83E-01
PEM (Grid) eHB (China)	1.6	1.48E-01	8.15E-01	6.09E-01	8.57E-02	1.43E-01	1.49E-01	1.21E-01	0.00E+00	1.00E+00	5.65E-01	0.00E+00	0.00E+00	9.85E-01	6.86E-01	7.82E-01	1.00E+00	9.03E-01	1.00E+00	1.00E+00
PEM (Grid) eHB (Germany)	1.7	4.55E-01	0.00E+00	4.10E-01	3.37E-01	4.52E-01	5.28E-01	4.13E-01	0.00E+00	1.00E+00	5.65E-01	3.21E-02	0.00E+00	1.00E+00	1.00E+00	1.00E+00	5.87E-01	1.00E+00	8.82E-01	8.13E-01
Biogas SMR HB (India)	1.8	9.93E-01	9.97E-01	9.91E-01	9.98E-01	9.98E-01	9.98E-01	9.97E-01	2.96E-01	9.00E-01	1.00E+00	0.00E+00	0.00E+00	8.68E-01	6.75E-01	7.39E-01	9.70E-01	6.61E-01	7.01E-01	7.83E-01
Biogas SMR HB (China)	1.9	9.93E-01	9.97E-01	9.91E-01	9.98E-01	9.98E-01	9.98E-01	9.97E-01	2.96E-01	9.00E-01	1.00E+00	0.00E+00	0.00E+00	9.85E-01	6.86E-01	7.82E-01	1.00E+00	9.03E-01	1.00E+00	1.00E+00
Direct Solution Mining (India)	2.1	3.69E-01	3.51E-01	0.00E+00	0.00E+00	9.95E-02	1.43E-01	1.54E-02	3.43E-01	9.19E-01	1.00E+00	8.68E-01	0.00E+00	8.81E-01	9.84E-01	9.45E-01	9.70E-01	7.33E-01	7.01E-01	7.83E-01
Direct Solution Mining (China)	2.2	3.69E-01	3.51E-01	0.00E+00	0.00E+00	9.95E-02	1.43E-01	1.54E-02	3.43E-01	9.19E-01	1.00E+00	6.17E-01	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
Indirect Solution Mining (India)	2.3	0.00E+00	0.00E+00	6.08E-01	5.96E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.18E-01	9.88E-01	3.14E-01	0.00E+00	8.81E-01	9.84E-01	9.45E-01	9.70E-01	7.33E-01	7.01E-01	7.83E-01
Indirect Solution Mining (China)	2.4	0.00E+00	0.00E+00	6.08E-01	5.96E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.18E-01	9.88E-01	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
Rock Salt Mining (India)	2.5	9.08E-01	9.49E-01	8.60E-01	8.65E-01	7.36E-01	8.23E-01	6.48E-01	9.90E-01	1.00E+00	1.00E+00	5.70E-01	0.00E+00	8.81E-01	9.84E-01	9.45E-01	9.70E-01	7.33E-01	7.01E-01	7.83E-01
Rock Salt Mining (China)	2.6	9.08E-01	9.49E-01	8.60E-01	8.65E-01	7.36E-01	8.23E-01	6.48E-01	9.90E-01	1.00E+00	1.00E+00	5.72E-01	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
DAC (India)	3.1	7.78E-01	9.57E-01	9.79E-01	6.13E-01	7.81E-01	6.75E-01	5.17E-01	0.00E+00	1.00E+00	1.00E+00	0.00E+00	0.00E+00	8.68E-01	6.75E-01	7.39E-01	9.70E-01	6.61E-01	7.01E-01	7.83E-01
DAC (China)	3.2	8.50E-01	9.57E-01	9.78E-01	6.46E-01	8.11E-01	7.22E-01	5.31E-01	0.00E+00	1.00E+00	1.00E+00	0.00E+00	0.00E+00	9.85E-01	6.86E-01	7.82E-01	1.00E+00	9.03E-01	1.00E+00	1.00E+00
DAC (Germany)	3.3	1.00E+00	8.26E-01	9.71E-01	7.41E-01	8.76E-01	8.43E-01	5.63E-01	0.00E+00	1.00E+00	1.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	5.87E-01	1.00E+00	8.82E-01	8.13E-01
MEA (India)	3.4	9.60E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.13E-01	9.94E-01	9.95E-01	9.57E-01	0.00E+00	8.68E-01	6.75E-01	7.39E-01	9.70E-01	6.61E-01	7.01E-01	7.83E-01
MEA (China)	3.5	9.60E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.13E-01	9.94E-01	9.95E-01	9.57E-01	0.00E+00	9.85E-01	6.86E-01	7.82E-01	1.00E+00	9.03E-01	1.00E+00	1.00E+00

Indexing		Normalised Objective Results																		
Spoke	ID	Global Warming Potential (GWP 100)	Ozone Depletion	Metal Resource Depletion	Freshwater Eutrophication Potential	Marine Eutrophication Potential	Acidification Potential (Terrestrial)	Water Use	Energy Demand	Energy Efficiency	Mass Efficiency	OpEx/Procurement Price	CapEx	Worker Health & Safety	Child Labour Risk	Forced Labour Risk	Utilisation of Hazardous Materials	Changes to Local Water Supply	Changes to Local Electricity Supply	Changes to Local Land Use
Wind (India)	4.1	9.80E-01	9.84E-01	1.13E-01	9.95E-01	9.77E-01	9.82E-01	9.84E-01	0.00E+00	1.00E+00	1.00E+00	6.15E-01	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
Solar (India)	4.2	9.55E-01	9.53E-01	0.00E+00	9.95E-01	9.68E-01	9.64E-01	9.58E-01	0.00E+00	1.00E+00	1.00E+00	6.15E-01	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
Bioenergy (India)	4.3	9.02E-01	5.72E-01	4.68E-01	9.80E-01	1.89E-01	7.19E-01	9.59E-01	0.00E+00	1.00E+00	1.00E+00	5.38E-01	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
Hydro (India)	4.4	9.93E-01	9.94E-01	8.35E-01	9.99E-01	9.91E-01	9.95E-01	9.96E-01	0.00E+00	1.00E+00	1.00E+00	5.38E-01	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
CHP, Lignite (India)	4.5	0.00E+00	9.61E-01	8.25E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	6.41E-01	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
CHP, Oil (India)	4.6	3.42E-01	0.00E+00	7.93E-01	9.93E-01	2.33E-01	7.98E-02	8.86E-01	0.00E+00	1.00E+00	1.00E+00	6.41E-01	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
CHP, Biogas (India)	4.7	8.40E-01	9.56E-01	6.89E-01	9.84E-01	8.98E-01	7.86E-01	9.64E-01	0.00E+00	1.00E+00	1.00E+00	5.38E-01	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
CHP, Natural Gas (India)	4.8	5.11E-01	6.13E-01	4.67E-01	9.95E-01	8.17E-01	8.97E-01	5.93E-01	0.00E+00	1.00E+00	1.00E+00	6.85E-01	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
Grid (India)	4.9	3.44E-01	9.16E-01	6.77E-01	7.04E-01	1.80E-01	5.06E-02	4.29E-01	0.00E+00	1.00E+00	1.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
CHP, Lignite (India)	5.1	3.20E-02	9.69E-01	8.32E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	4.94E-01	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
CHP, Oil (India)	5.2	3.64E-01	2.13E-01	8.01E-01	9.93E-01	2.33E-01	7.97E-02	8.86E-01	0.00E+00	1.00E+00	1.00E+00	4.94E-01	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
CHP, Biogas (India)	5.3	8.57E-01	9.68E-01	7.24E-01	9.85E-01	9.06E-01	8.03E-01	9.67E-01	0.00E+00	1.00E+00	1.00E+00	3.50E-01	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
CHP, Natural Gas (India)	5.4	5.27E-01	6.95E-01	4.88E-01	9.95E-01	8.17E-01	8.97E-01	5.93E-01	0.00E+00	1.00E+00	1.00E+00	5.56E-01	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
Natural Gas, Furnace (India)	5.5	0.00E+00	0.00E+00	6.81E-01	9.93E-01	7.89E-01	8.30E-01	9.62E-01	0.00E+00	1.00E+00	1.00E+00	3.17E-01	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
Biomass, Furnace (India)	5.6	7.53E-01	8.54E-01	0.00E+00	9.41E-01	2.92E-01	6.59E-01	8.15E-01	0.00E+00	1.00E+00	1.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00

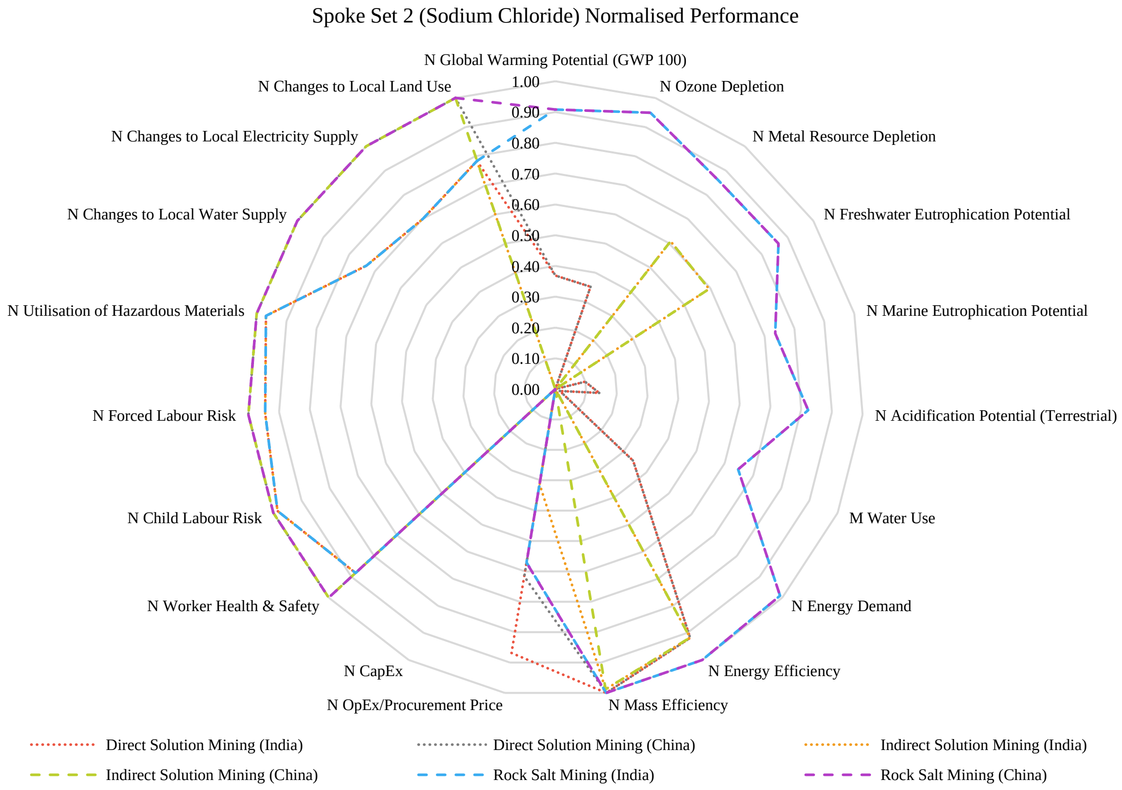


Figure 6-23 – Relative performance of spokes within set 2 against the proof-of concept indicators (normalised).

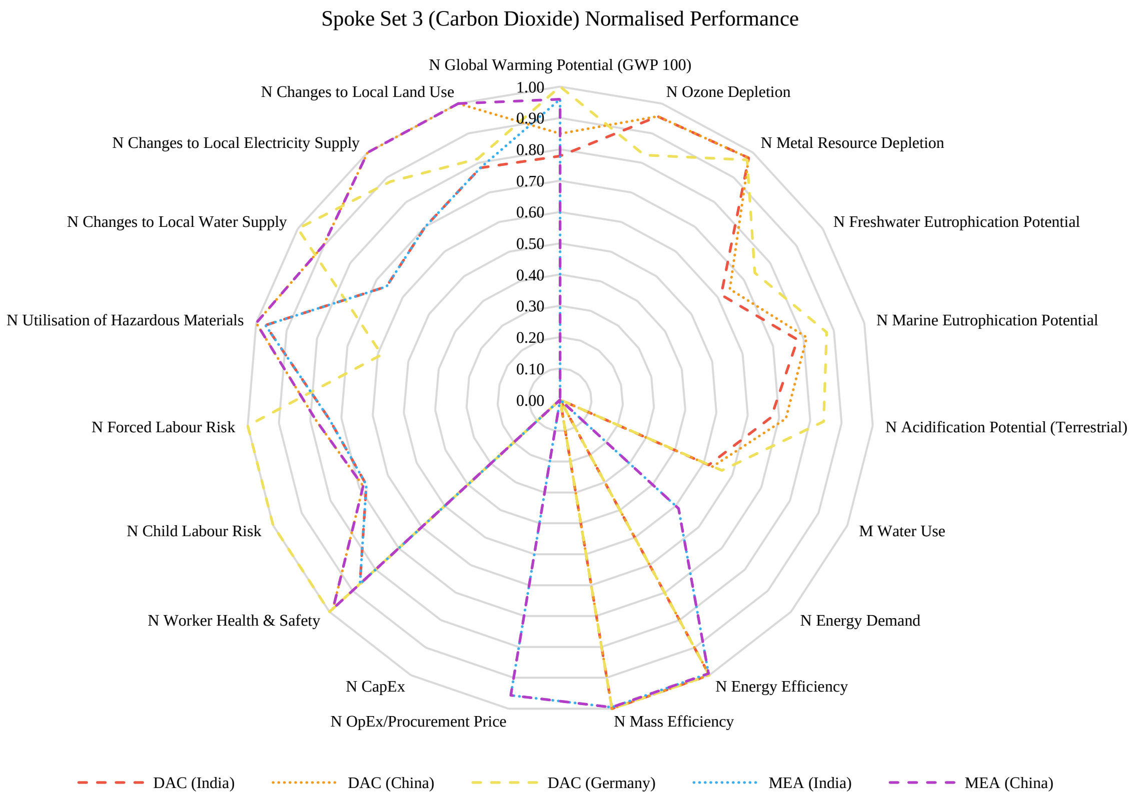


Figure 6-24 – Relative performance of spokes within set 3 against the proof-of concept indicators (normalised).

Figure 6-24 details the performance of alternate CO_2 capture routes, reflecting the purple component of Unilever's Carbon Rainbow. Across the environmental indicators, the three DAC spokes have comparable values, as expected. Although, some rank reversals are observed between GWP and ozone depletion. Overall, DAC in Germany offers the best performance, followed closely by DAC in China. This result offers an interesting comparison between European and Asian industrial nations; the variation is largely attributable to the grid mix providing energy within the DAC systems. In contrast to the environmental indicators, the MEA routes offer better economic performance, particularly regarding OpEx (35.3 £/tonne (MEA) vs 812 £/tonne (DAC)). This difference is partially explained by the electricity demand per tonne of CO_2 captured (6,930 kWh / tonne (DAC) vs 3,380 kWh / tonne (MEA)). While such a gulf in price and energy demand is exacerbated by the lower TRL of DAC, the systems' respective inlet CO_2 concentrations and resulting thermodynamic underpinnings ensure that parity will never be reached.

In parallel to these more micro-scale indicator specific takeaways, on a macro-level, the spokes assessed for the provision of carbon dioxide appear more visually competitive than those of the other two material-oriented spoke sets; reflecting more frequent rank reversal between examined alternatives. However, when this is compared in terms of each spoke sets MAD across the 19 assessed indicators (using Equation 6-7), the carbon dioxide set is quantitatively revealed to have slightly larger performance differentials (0.197 vs 0.177) (see Table 6-31). This fact offers insights into data communication strategies for the framework; while the visual representation allows for the identification of preferentially performing alternatives in most situations, the degree of performance differentiation can only be reliably interpreted by examining the data with analytical tools such as MAD. LCA's position as a data intensive field necessitates this type of systematic and repeatable results communication strategy, minimising scope for divergent interpretation by different practitioners.

Table 6-31 – Mean absolute difference (MAD) observed within each spoke sets across each assessed impact indicator. Calculated using Equation 6-7 and averaged as a mean for each spoke set in the right most column.

Spoke Set	MAD of Observed Normalised Indicator Values																			Average Spoke Set MAD
	N Global Warming Potential (GWP 100)	N Ozone Depletion	N Metal Resource Depletion	N Freshwater Eutrophication Potential	N Marine Eutrophication Potential	N Acidification Potential (Terrestrial)	M Water Use	N Energy Demand	N Energy Efficiency	N Mass Efficiency	N OpEx/Procurement Price	N CapEx	N Worker Health & Safety	N Child Labour Risk	N Forced Labour Risk	N Utilisation of Hazardous Materials	N Changes to Local Water Supply	N Changes to Local Electricity Supply	N Changes to Local Land Use	
1	0.317	0.199	0.329	0.379	0.352	0.341	0.351	0.146	0.049	0.215	0.054	0.000	0.059	0.063	0.047	0.079	0.129	0.136	0.104	0.176
2	0.321	0.344	0.326	0.324	0.305	0.334	0.284	0.364	0.036	0.005	0.222	0.000	0.059	0.008	0.027	0.015	0.134	0.150	0.108	0.177
3	0.076	0.438	0.468	0.320	0.395	0.358	0.258	0.246	0.003	0.002	0.459	0.000	0.059	0.102	0.077	0.127	0.131	0.125	0.099	0.197

The MAD results contained within Table 6-31 offer additional insights beyond the evaluation of results communication strategy. Generally, it is shown that the environmental indicators exhibit the greatest performance variations, and therefore MAD, of the three assessment strands ($\overline{MAD}_{LCA} = 0.325$). The economic ($\overline{MAD}_{TEA} = 0.120$) and societal ($\overline{MAD}_{SIA} = 0.088$) strands show notable smaller degrees of divergence, with societal indicators varying the least. Reviewing the system boundaries for the proof-of-concept assessment reveals a potential causal factor; the system boundaries. The LCA strand evaluates a full cradle-to-gate scope, whereas the TEA examines a more constrained system boundary. Due to the focus on the framework's applicability to FMCG value chains, the price related TEA indicators are evaluated based on purchase price of the spokes reference flow from that route, aligning with the reality of FMCG companies' operations. Consequently, a narrower range of indicator results can be reasonably expected due to the economically competitive nature of the routes; selling the same product in the same quantities. Routes performing optimally environmentally or socially can only charge a certain amount more than the less sustainable alternatives if they are to command a meaningful market share (unless severe carbon tariffs come to fruition). The social indicators' position as the lest divergent indicator results within each spoke set speaks clearly to the national resolution on which the risk of negative impact is assessed. If more granular, process or sector specific characterisation models are developed, greater accuracies and degrees of differentiation would be observed in the strand's intra-spoke set results. Furthermore, for most spoke sets two or more alternatives are assessed in both China and India, resulting in identical national level SIA results; a notable current limitation of the framework stemming from the work within Chapter 5.

Figure 6-25 displays the relative performance of the electricity provision spoke set. Immediately, it is apparent that the social indicators deliver identical scores for all alternatives. This is again a consequence of the national level focus of the SIA characterisation models developed in Chapter 5, coupled with the purely domestic sourcing within the proof of concept. Economically the alternatives are largely comparable, the most significant differences reside in the OpEx indicator. Provision from the Indian grid is the most expensive of the options, 2.5 times the average cost per kWh of technology specific alternatives purchased directly (£0.11 per kWh as opposed to around £0.04 per kWh for the other alternatives. This initially counterintuitive fact can be explained by several localised factors currently acting to inflate the cost of Indian grid electricity [303];

1. Long term power purchase agreements imposed by the generating parties (typically 25 years)
2. Rigid contracts and underutilisation of capacity that prevents dynamic pricing based on availability
3. Distribution issues affecting installed renewable capacity
4. Inadequate and inefficient infrastructure preventing optimal dispatch of generated energy
5. Operational inefficiencies and poor financial health of distribution companies

These factors combine to raise the price of grid electricity for both industrial and regular consumers. The result is a significant price advantage for independent generation feeding the Hou process. While incurring CapEx, it is assumed that this on-site electricity generation would be subcontracted to an external organisation in favour of slightly higher OpEx, accounting for the contractor's profit margin and ROI.

In terms of the environmental indicators, the results are difficult to visually interpret as a result of many rank reversals, supporting the framework's deployment of MCDM in these multivariate problems. However, some clear insights are generated prior to ranking of alternatives performance through AHP-TOPSIS. For instance, hydroelectric generation is revealed to be the best performer across LCA indicators, achieving the highest (best) score in all cases. This should perhaps be unsurprising following the case study examining energy generation impacts by source within Section 6.6.3.1.3 (and more specifically Table 6-25), in which hydro was the best performing alternative out of all assessed grid mix contributors. Notably poor performers include; lignite based CHP and the Indian grid mix (reflecting the 78.1% share of fossil-based production).

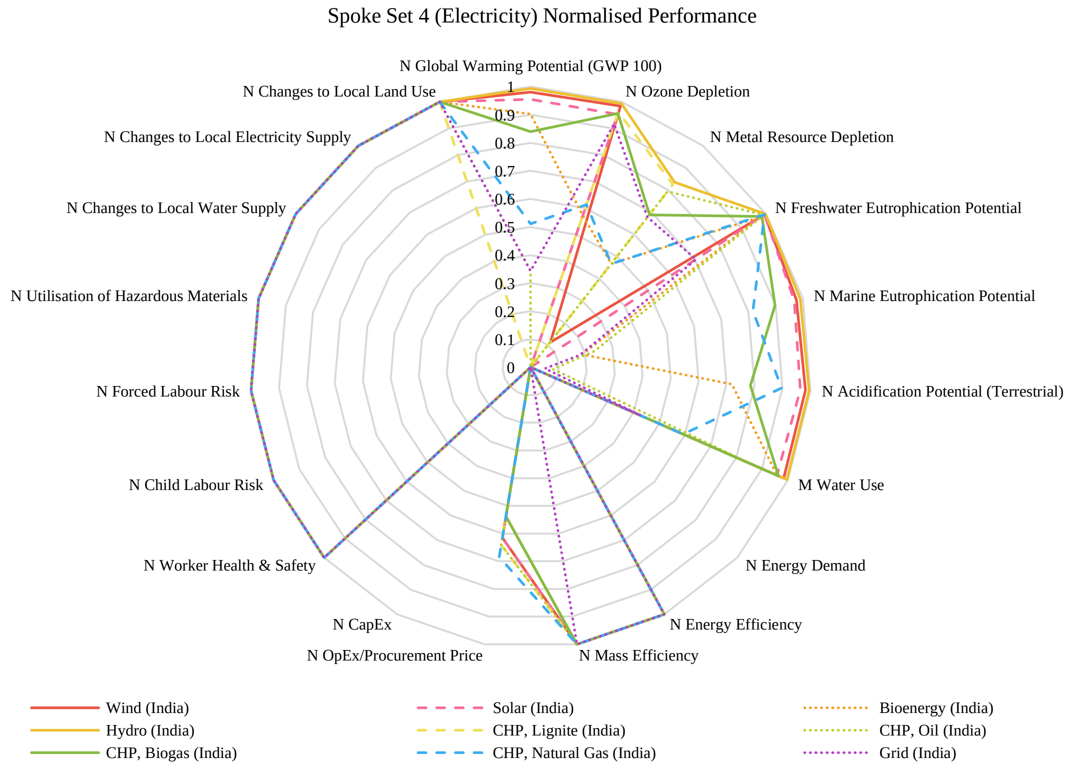


Figure 6-25 – Relative performance of spokes within set 4 against the proof-of concept indicators (normalised).

The impact indicator performance observed within the final spoke set, process heat provision, is detailed in Figure 6-26. Several of the generation methods utilise the same technology as spokes within the electricity provision set, resulting in similarities between the two radar plots (Figure 6-25 and Figure 6-26). Again, owing to the national level assessment of social impact risk, and solely domestic provision, all alternatives exhibit the same SIA indicator values.

The aforementioned similarity in indicator results between heat and electricity provision spoke sets is most apparent within the TEA. The OpEx performance is more favourable for the CHP spokes compared to the individual heat or electricity generation methods; a consequence of greater energy recovery performance (note; energy efficiency is quantified based on electrical inputs to the spokes, excluding energy stored in combustion fuels). The allocation procedure for the CHP spokes is based on energy ($kWh_{electricity}$ = 1 $kWh_{thermal}$) as suggested by the GCI, a convenient solution made possible by comparable functional units. At the extremes of performance envelopes, class leading CHP is more than twice as efficient as large-scale thermal power plants (98% versus 45% energy recovery [304]), resulting in lower relative impacts (both environmentally and economically).

CHP's efficiency advantage is reflected strongly within the alternative's LCA indicator performance. Biogas fed CHP is revealed through the impact profiles to be the best option, realising the combined benefits of elevated efficiency and biogenic carbon source. Natural gas fed CHP is a relatively distant second, only achieving the best performance in a single environmental factor (acidification potential), with no significantly poor performance in any given LCA indicator. Lignite fed CHP is the worst performer environmentally, reflecting in the impact results its position as the lowest grade of coal [305]. Because of its lower heating value and elevated moisture content, a significantly larger amount of lignite is required to generate 1 kWh than for higher grade alternatives (e.g. anthracite). However, with significant lignite deposits present in India (Tamil Nadu, Puducherry, Kerala, Gujarat, Rajasthan and Jammu and Kashmir regions), and its widespread use, it is selected as the most representative coal type for evaluation within the proof-of-concept assessment [306].

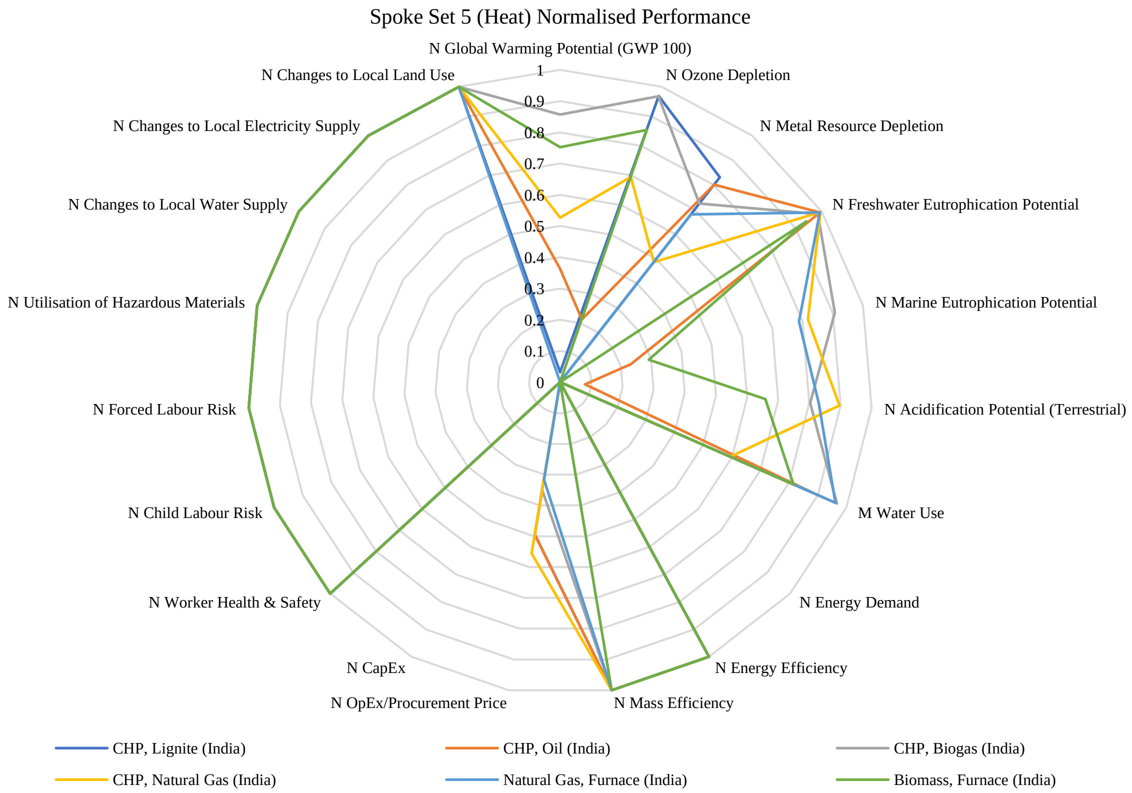


Figure 6-26 – Relative performance of spokes within set 5 against the proof-of concept indicators (normalised).

6.7.3 AHP-TOPSIS Derived Spoke Scores

With the objective and intra-set normalised results calculated for each of 19 indicators across all 35 examined spokes, their subjective sustainability scores can be calculated. These overall scores are the first integration of decision maker value choices and the objective indicator values derived from data. They combine the performance of each spoke relative to their constituent set, and the decision maker value choice derived indicator weightings. As discussed in Section 6.6.2, the proof-of-concept study applies an equal weighting (~0.05263) to provide a 'cleaner' basis on which the framework's efficacy can be evaluated. The methodological procedure for calculating the AHP weightings is given in Section 4.5.3.5, with the methodology for calculating spokes' overall score detailed in Section 4.5.2.4. Table 6-32 to Table 6-36 show each of the sets and their constituent spokes subjective sustainability scores. As with the normalisation procedures, higher scores indicate preferable performance.

Table 6-32 – Subjective sustainability scores for spoke set 1.

Ammonia Spoke Set Results			
Indexing		AHP-TOPSIS Scores	
Spoke	Ref.	Overall Score	Local Ranking
Biogas SMR HB (China)	1.9	0.8628	1
SMR HB (China)	1.2	0.8535	2
Biogas SMR HB (India)	1.8	0.7968	3
SMR HB (India)	1.1	0.7889	4
PEM (Wind) eHB (China)	1.4	0.6705	5
PEM (Wind) eHB (India)	1.3	0.6457	6
PEM (Grid) eHB (Germany)	1.7	0.3972	7
PEM (Grid) eHB (China)	1.6	0.3693	8
PEM (Grid) eHB (India)	1.5	0.3106	9

Table 6-33 – Subjective sustainability scores for spoke set 2.

Sodium Chloride Spoke Set Results			
Indexing		AHP-TOPSIS Scores	
Spoke	Ref.	Overall Score	Local Ranking
Rock Salt Mining (China)	2.6	0.8950	1
Rock Salt Mining (India)	2.5	0.8156	2
Direct Solution Mining (India)	2.1	0.3487	3
Direct Solution Mining (China)	2.2	0.3381	4
Indirect Solution Mining (China)	2.4	0.2987	5
Indirect Solution Mining (India)	2.3	0.2882	6

Table 6-34 – Subjective sustainability scores for spoke set 3.

Carbon Dioxide Spoke Set Results			
Indexing		AHP-TOPSIS Scores	
Spoke	Ref.	Overall Score	Local Ranking
DAC (Germany)	3.3	0.6371	1
DAC (China)	3.2	0.6334	2
DAC (India)	3.1	0.5951	3
MEA (China)	3.5	0.3762	4
MEA (India)	3.4	0.3504	5

Table 6-35 – Subjective sustainability scores for spoke set 4.

Electricity Provision Spoke Set Results			
Indexing		AHP-TOPSIS Scores	
Spoke	Ref.	Overall Score	Local Ranking
Hydro (India)	4.4	0.9474	1
CHP, Biogas (India)	4.7	0.8726	2
Wind (India)	4.1	0.7744	3
Solar (India)	4.2	0.7439	4
CHP, Natural Gas (India)	4.8	0.7064	5
Bioenergy (India)	4.3	0.6620	6
CHP, Oil (India)	4.6	0.5064	7
Grid (India)	4.9	0.4624	8
CHP, Lignite (India)	4.5	0.3894	9

Table 6-36 – Subjective sustainability scores for spoke set 5.

Heat Provision Spoke Results			
Indexing		AHP-TOPSIS Scores	
Spoke	Ref.	Overall Score	Local Ranking
CHP, Biogas (India)	5.3	0.9049	1
CHP, Natural Gas (India)	5.4	0.7517	2
Biomass, Furnace (India)	5.6	0.6010	3
Natural Gas, Furnace (India)	5.5	0.5937	4
CHP, Oil (India)	5.2	0.5494	5
CHP, Lignite (India)	5.1	0.3996	6

The average range of subjective sustainability scores observed across the spoke sets is 0.502 (0.552, 0.607, 0.287, 0.558, and 0.505 respectively). Considering the methodologically applied bounds of 0 and 1, this shows a reasonable scoring distribution resulting in meaningful differentiation of performance. However, the range alone cannot rule out the effects of clustered scores with one significant outlier. To this end, the standard deviation (σ) for each spoke set's scores is also evaluated, determining the average distance of scores from the mean. Through this, a value of $\bar{\sigma} \approx 0.201$ (0.219, 0.279, 0.143, 0.188, and 0.174 for the five sets respectively) is revealed. Given the maximum range of 1, this is satisfactory to rule out tight score grouping in all sets (confirmed visually by Figure 6-27).

It is also revealed, perhaps obviously, that the number of alternatives within each set moderately correlates (r = 0.570) with the observed range. As the number of alternatives within a set increase, the likelihood of a very good or very poor option being present increases. The same correlation is not observed between standard deviation and number of constituent spokes (r = 0.195), validating that set size does not restrict the average dispersion of resulting subjective sustainability scores. This supports the broad application of the framework to assessments with either few or plentiful alternatives for each feedstock type.

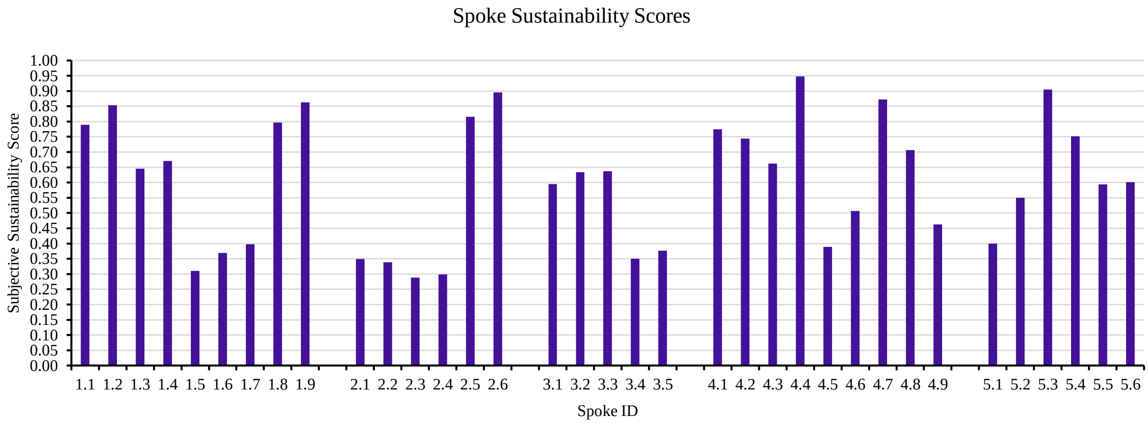


Figure 6-27 – Subjective sustainability scores of all assessed spokes.

Figure 6-27 shows the subjective sustainability scores of each evaluated spoke, grouped into their respective sets. Each of these sets contains an option possessing an overall score in excess of 0.85, with the exception of set 3 (CO_2 capture as a feedstock). This lack of a strong performing CO_2 feedstock procurement option (spoke set 3) can be attributed to the examination of only two technology types. This is compounded by their diametrically opposing performance profiles across assessment strands. DAC performs well in the LCA strand but exhibits very poor performance across the TEA indicators (particularly OpEx) as a consequence of energy demand and lower relative TRL. The opposite is true for MEA capture, with worst in set LCA indicator performance and best in set TEA performance. The comparatively low range (0.287) observed in set 3 suggests that the MDCM and aggregation procedures are successfully balancing trade-offs. This is further confirmed by altering the strand weightings (W_i) as shown in Figure 6-28; $W_{LCA} = 0.692$, $W_{TEA} = 0.231$, and $W_{SIA} = 0.077$ (achieving *C.R.= 0*, confirming validity of the input pairwise comparisons).

Strands	LCA	TEA	SIA
LCA		3	9
TEA	1/3		3
SIA	1/9	1/3	

Consistency Ratio	0

Figure 6-28 – MCDM configuration for the evaluation of methodological efficacy when considering spoke set 3.

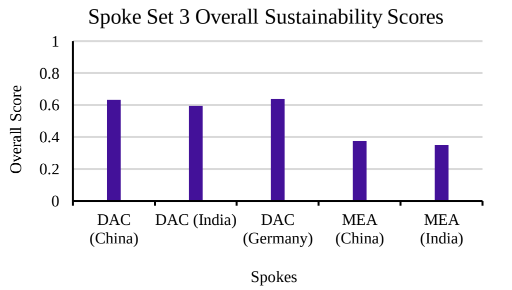


Figure 6-29 - Scores of set 3's spokes with adjusted strand MCDM weights

This change in weighting should theoretically increase the range of the scores observed in spoke set 3 as the MEA routes strong economic performance no longer has the same strong compensatory effect on the poor LCA performance. Revised spoke scores resulting from this weighting change, shown in Figure 6-29, confirm this hypothesis. The original range of 0.287 increases to 0.584, strongly recommending DAC for deployment in a Hou process oriented soda ash value chain, due to the strong decision maker indicated preference for performance maximisation in the LCA strand.

Together, Sections 6.7.2 and 6.7.3 verify the efficacy of the local objective assessment and subjective sustainability scoring of spokes within their sets. The objective and intra-set normalised data follows expectations laid out in Chapter 4 in terms of both values and behaviour. Furthermore, the delivery of each spoke's impact results (across all 19 indicators barring CapEx) relative to their respective local functional unit, confirms their operability as stand-alone assessments that can be re-purposed in subsequent hub and spoke assessments including that reference product. Furthermore, the normalisation procedures and aggregation of indicator scores to a single subjective sustainability score delivers an easily interpretable metric for use by non-practitioners. Ultimately, this points to significant efficacy in the support of industrial decision making, delivering easily interpretable and distinct scoring profiles across each spoke set. The adoption of continuous scoring scales is also shown to be possible within all assessment strands, delivering much more granular insights than their discrete reference scale alternatives; such as those proposed by the triple helix framework [7].

6.7.4 Scoring Profile of Aggregated Value Chains

With the spokes and spoke sets defined and evaluated in isolation, their aggregation into an assessment of the full value chain can be approached. The first step towards this is the definition of all possible value chain permutations. In the proof-of-concept study, MS Excel's Power Query tool was used to accomplish this while reducing practitioner workload. Given the number of permutations present, manual compilation would be time intensive, with the repetitive task also likely to induce human error. With a single hub, five spoke sets, and a total of 35 independent spokes present within the proof-of-concept assessment (9, 6, 5, 9, 6 distribution), 14,580 permutations are present (calculated using Equation 4-13).

Initially, the list of all permutations and their active spoke I.D.s is compiled in the format of Table 4-11 and Table 4-12, including the objective and normalised indicator results. Each of the value chain's objective indicator results are subsequently aggregated to deliver an overall cradle-to-gate result using Equation 4-14 for the LCA and TEA indicators, and Equation 4-15 for the SIA indicators. With these objective results generated for each of the 14,580 permutations, comparable to those seen in traditional assessments, their subjective ranking based on the decision makers MCDM inputs can be approached. As discussed in Section 4.5.3.8 of Chapter 4, this is based on the active spokes' subjective sustainability score. The value chain's 'overall subjective sustainability score' for each permutation is evaluated through Equation 4-16, again delivering a value between 0 and 1 where higher scores are preferable (as seen with the local spoke scoring).

By plotting successive value chain permutation's ranks against their overall subjective sustainability scores, the graph shown in Figure 6-30 is obtained. This exhibits very steep gradients at the high and low scoring extremes, with a significantly lesser gradient around the average score. As observed with the local intra-spoke set results, the full extent of the scoring range is not utilised. Although, given that the overall value chain scores are derived from the spoke scores, this is to be expected. The realised range between the proof-of-concept study's best and worst performing value chain permutations is 0.501 (0.849 – 0.348), delivering a broad enough distribution for the drawing of meaningful conclusions.

The general form of the scoring profile supports the frameworks use as a tool to support decision making within the FMCG industry. Given that only a small percentage of permutations attain overall subjective sustainability scores lying in the >0.8 range (85 of 14,580, or 0.583%), this is a highly effective methodology for screening out sub-optimal value chain options. With further application of the framework to increase behavioural understanding, and use based consultation with FMCG based industrial decision makers, a cut-off scoring value or percentile may be identified. Such a development would standardise the screening application of the framework for use in less granular assessments, selecting value chain permutations for further analysis on a consistent and repeatable basis while accounting for practical constraints such as available person-hours. A cut-off approach is less relevant to non-screening framework applications involving highly resolved data; in these cases, the best performing value chain is likely to be selected directly due to decreased uncertainty within the impact indicator results.

In the event that a given assessment generates tightly grouped scores for all permutations, this is indicative of spoke sets exhibiting one of two typologies;

1. Very little differentiation between assessed spokes
2. Highly varied performance with compensatory effects

The causation of the score grouping can be determined through a AHP oriented sensitivity analysis. If the observed scoring range does not change significantly as indicator weightings are varied, typology 1 is present. If the overall and local scores do change notably with the AHP derived weightings, performance differentials do exist but are neutralised by the initial MCDM configuration (as observed for the DAC spoke set within the Section 6.7.3).

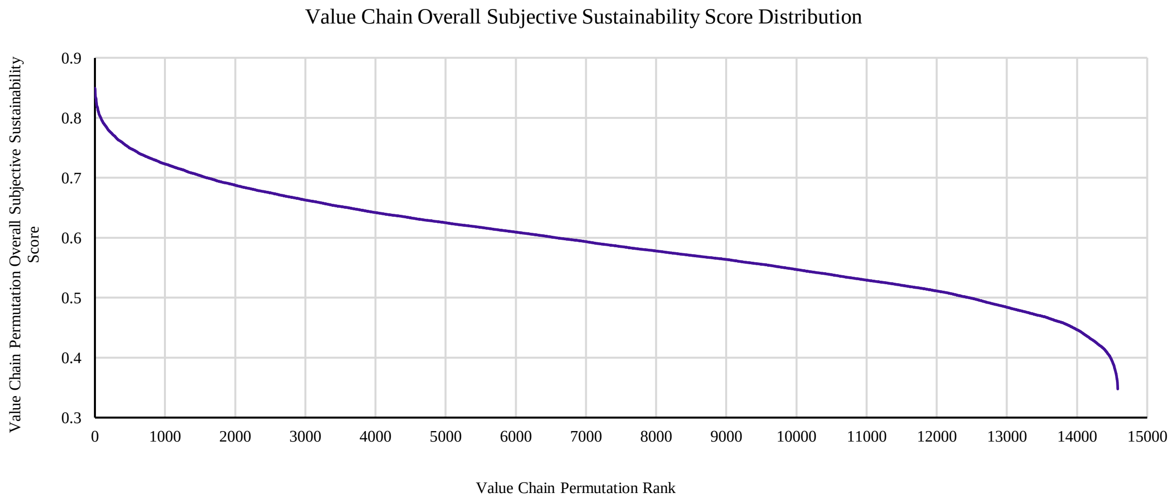


Figure 6-30 – Overall subjective sustainability score achieved vs permutation rank.

Returning to consideration of the scoring profile for the proof-of-concept study (Figure 6-30), the curve exhibits what initially appears to be normally distributed data on the macro-level, with the majority of permutation scores falling around a mean value at the point of lowest gradient. Behaviour of this type was expected. Scores falling within the upper and lower percentiles must primarily utilise the best and worst performing spokes from each set, constituting a very limited number of permutations. In contrast, scores closer to the mean can either utilise uniformly mediocre spokes from each set, or a mixture of high and low performance spokes. Naturally, this results in a probability bias towards scores approximating the mean.

By carving the full range of possible scoring values (0 - 1) into 40 equally sized intervals, the frequency distribution can be evaluated. Scoring increments of 0.025 were selected to deliver reasonable resolution while being broad enough to smooth micro-level local frequency variations. This frequency data is then overlaid with a normal distribution (Equation 6-10) for comparison.

Equation 6-10 – Generation of a normal distribution curve to overlay on to the proof-of-concept data. Where, x is the overall value chain sustainability score achieved, μ is the mean, and σ is the standard deviation.

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

As seen by Figure 6-31, the scoring frequency distribution does closely follow a normal distribution (r = 0.999). The mean overall subjective sustainability score (μ) of 0.588 is revealed, with a standard deviation of 0.088. No notable skew is identified. A mean score in close proximity to the scoring scale's midpoint indicates good performance of the procedure used to normalised indicator performance within each spoke set. Due to the anchoring of a zero score to the worst performing alternative for each indicator, and a score of 1 to a hypothetical target scenario (e.g. *GWP* = 0 kg CO_2-eq / FU), the scale is dynamic and adapts to the range of performance profiles present in a given assessment. Rigid positioning of both the upper and lower normalisation bounds would deliver less certain insights as the impacts observed for the assessed alternatives are unlikely to command the same breadth of scoring range, and therefore differentiation.

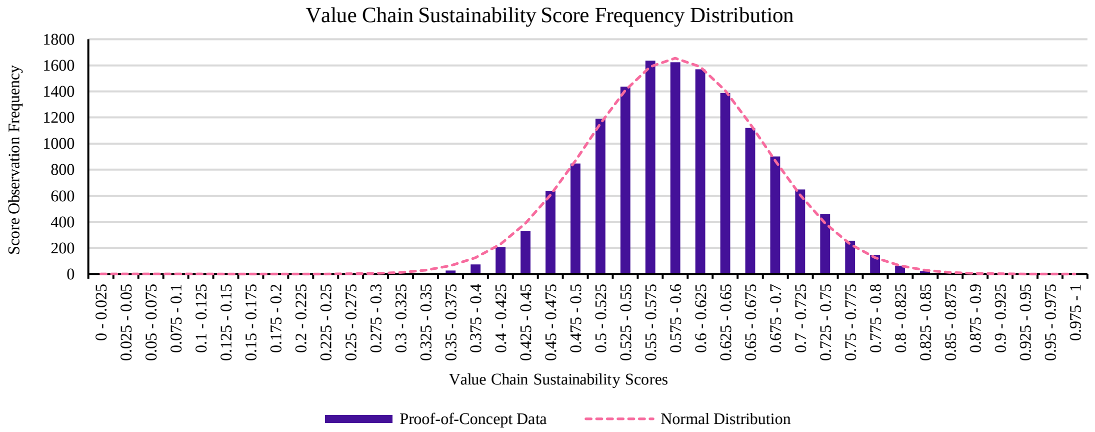


Figure 6-31 – Frequency distribution of the proof-of-concept study's overall subjective sustainability score with an overlaid normal distribution function.

The standard deviation of the distribution (σ = 0.088) indicates that ~95% of the scores fall between 0.412 and 0.764 ($\mu \pm 2\sigma$), a consequence of the approximately normal behaviour. When compared to the observed score range (0.348 - 0.849) the best performing permutations are far enough removed from the $\mu + 2\sigma$ value to dismiss all permutations with an overall subjective sustainability score of < $\mu + 2\sigma$ (<0.764) from further consideration. Based on this approach a total of 326 permutations (2.24% of the initial total) remain. Even if employing the framework as a screening assessment, the chances of reasonable degrees of uncertainty causing the true best alternative below this threshold is exceedingly small.

6.7.5 Examination of Assessment Results (Interpretation)

Given the quantity and high level nature of the data contained within Figure 6-30 and Figure 6-31, alternate approaches to interpretation are required in order to act upon the assessment's outputs. As a result of the modularity of the hub and spoke framework, this can be tackled with more dexterity than is observed in traditional assessments. While providing stakeholders with recommended value chains, analogous to the interpretation phase realised through existing LCA methodologies, spokes selection frequency within their local sets can also be examined. The methodologies compartmentalisation of LCI and LCIA phases is therefore seen to enable extraction of more nuanced insights; a fact confirmed by the following parallel evaluation of both overall recommendations and local spoke set performance.

6.7.5.1 Best Performing Value Chain Permutations

Clearly, the initial set of permutations (*n*=14,580) must be significantly reduced to deliver direct and exercisable utility to a FMCG company. Therefore, the objective indicator values and overall subjective scores are presented for the proof-of-concept study's five best performing permutations within Table 6-37 and Table 6-38 respectively. These value chain recommendations suggests that the optimal India based soda ash production value chain utilising the Hou process and available feedstocks employs; ammonia from biogas fed SMR HB in China, sodium chloride from rock salt mining in China, CO_2 from direct air capture in Germany, domestic hydroelectricity, and heat purchased from a biomass fed CHP plant. Such a value chain attains a promising overall subjectivity score of 0.8494. Examining the following four recommendations, the overall subjective sustainability scores are closely grouped, reaching a maximum deviation from the top-ranking permutation of only 0.008. Given this proximity, and the fact that the proof-of-concept study does not include aspects such as transport impacts (important for the shipping of DAC captured CO_2 from Germany to India), a more detailed iteration of the assessment would be needed to verify the ranking order of these initially selected permutations.

However, even when applied at this screening level, the framework demonstrates its effectiveness in reducing a large set of possible permutations to a curated group of promising performers. From here, FMCG companies can more accurately allocate resources to more granular assessments, potentially entering joint development agreements (JDA), or R&D efforts. Alternatively, where a smaller group of alternatives are present, considerations such as transport impacts can be incorporated to deliver much more accurate LCIA results, negating the ned for further assessment.

Table 6-37, detailing the active spoke I.D.'s for the five best performing permutations, reveals uniform selection from sets 2, 4, 5. This suggests that the overall subjective sustainability scores is most sensitive to spoke selection in these sets. By consulting Figure 6-27 (the spokes local sustainability scores), the cause of this sensitivity becomes clear; sets 2, 4, and 5 exhibit the largest scoring differences between their best and second-best performing spokes (0.079, 0.075, and 0.153 respectively). Consequently, value chains utilising any spoke other than the best performing alternative in these sets are at a significant disadvantage when calculating the overall subjective sustainability score. Such a large performance differential between set 5's top two alternatives suggest that spoke 5.3 will be present in a significant majority of permutations residing in the upper scoring percentiles (evaluated in more detail within Section 6.7.5.2).

The inverse is true for the sets with varied active spoke selection within the five top scoring permutations. Sets 1 and 3 have a best to second-best subjective sustainability score deviation of just 0.009 and 0.004 respectively.

Table 6-37 – Five best performing value chain permutations within the proof-of-concept assessment with their active spoke IDs for each set, spoke names, subjective spoke scores, and overall subjective sustainability scores.

Value Chain Ranking	Value Chain Permutation ID	NH_3 Source			NaCl Source			CO_2 Source			Electricity Generation			Heat Generation			Overall Subjective Sustainability Score
		ID	Spoke Name	Spoke Score	ID	Spoke Name	Spoke Score	ID	Spoke Name	Spoke Score	ID	Spoke Name	Spoke Score	ID	Spoke Name	Spoke Score	
1	14439	1.9	Biogas SMR HB (China)	0.8628	2.6	Rock Salt Mining (China)	0.8950	3.3	DAC (Germany)	0.6371	4.4	Hydro (India)	0.9474	5.3	CHP, Biogas (India)	0.9049	0.8494
2	14385	1.9	Biogas SMR HB (China)	0.8628	2.6	Rock Salt Mining (China)	0.8950	3.2	DAC (China)	0.6334	4.4	Hydro (India)	0.9474	5.3	CHP, Biogas (India)	0.9049	0.8487
3	3099	1.2	SMR HB (China)	0.8535	2.6	Rock Salt Mining (China)	0.8950	3.3	DAC (Germany)	0.6371	4.4	Hydro (India)	0.9474	5.3	CHP, Biogas (India)	0.9049	0.8476
4	3045	1.2	SMR HB (China)	0.8535	2.6	Rock Salt Mining (China)	0.8950	3.2	DAC (China)	0.6334	4.4	Hydro (India)	0.9474	5.3	CHP, Biogas (India)	0.9049	0.8468
5	14331	1.9	Biogas SMR HB (China)	0.8628	2.6	Rock Salt Mining (China)	0.8950	3.1	DAC (India)	0.5951	4.4	Hydro (India)	0.9474	5.3	CHP, Biogas (India)	0.9049	0.8410

Table 6-38 – Five best performing value chain permutations within the proof-of-concept assessment with their overall objective impact indicator results inclusive of the hub and all active spokes.

Value Chain Ranking	Value Chain Permutation ID	Objective Indicator Results																	
		Global Warming Potential (GWP 100) (kg CO_2-eq. / FU)	Ozone Depletion (kg CFC-11-eq. / FU)	Metal Resource Depletion (kg Cu-eq. / FU)	Freshwater Eutrophication Potential (kg P-eq. / FU)	Marine Eutrophication Potential (kg N-eq. / FU)	Acidification Potential (Terrestrial) (kg PSO_2-eq. / FU)	Water Use (m^3 / FU)	Energy Demand (MJ / FU)	Energy Efficiency (%)	Mass Efficiency (%)	OpEx/Procurement Price (2022 GBP / FU)	CapEx (2022 GBP / FU)	Worker Health & Safety (N.D.)	Child Labour Risk (N.D.)	Forced Labour Risk (N.D.)	Utilisation of Hazardous Materials (N.D.)	Changes to Local Water Supply (N.D.)	Changes to Local Electricity Supply (N.D.)	Changes to Local Land Use (N.D.)
1	14439	2.47E+02	1.15E-05	6.47E+01	2.09E-01	4.92E-01	1.94E+00	5.73E+00	1.43E+04	9.28E+01	9.91E+01	8.31E+02	2.77E+00	5.43E-01	6.59E-01	7.48E-01	4.51E-01	6.01E-01	2.31E-01	6.50E-01
2	14385	2.59E+02	1.02E-05	6.45E+01	2.18E-01	5.09E-01	2.05E+00	5.78E+00	1.43E+04	9.28E+01	9.91E+01	8.31E+02	2.77E+00	5.41E-01	6.12E-01	7.13E-01	4.84E-01	5.89E-01	2.36E-01	6.73E-01
3	3099	8.69E+02	1.15E-05	6.45E+01	2.06E-01	4.88E-01	1.90E+00	6.11E+00	1.43E+04	9.28E+01	9.91E+01	7.99E+02	2.77E+00	5.43E-01	6.59E-01	7.48E-01	4.51E-01	6.01E-01	2.31E-01	6.50E-01
4	3045	8.81E+02	1.02E-05	6.43E+01	2.15E-01	5.05E-01	2.02E+00	6.16E+00	1.43E+04	9.28E+01	9.91E+01	7.99E+02	2.77E+00	5.41E-01	6.12E-01	7.13E-01	4.84E-01	5.89E-01	2.36E-01	6.73E-01
5	14331	2.65E+02	1.02E-05	6.45E+01	2.21E-01	5.17E-01	2.10E+00	5.80E+00	1.43E+04	9.28E+01	9.91E+01	8.31E+02	2.77E+00	5.27E-01	6.11E-01	7.07E-01	4.82E-01	5.59E-01	2.22E-01	6.46E-01

Consequently, utilisation of the second best spoke from these sets results in a relatively small increase in impact indicator results, and therefore, the overall subjective sustainability score of the value chain. In fact, when examining the spoke selection within set 3, all of the DAC routes assessed are present. With a range of local scores of just 0.042 across the three geographically differentiated alternates (China, India, and Germany), the practitioner and FMCG company gain the insight that deployment location is not a significantly sensitive factor in DAC spoke performance. However, it also reveals that the point source MEA based route is unlikely to contribute to a strongly performing value chain, reflected through its lack of selection, advising decision makers against potential expenditure of capital and employee time on further examination.

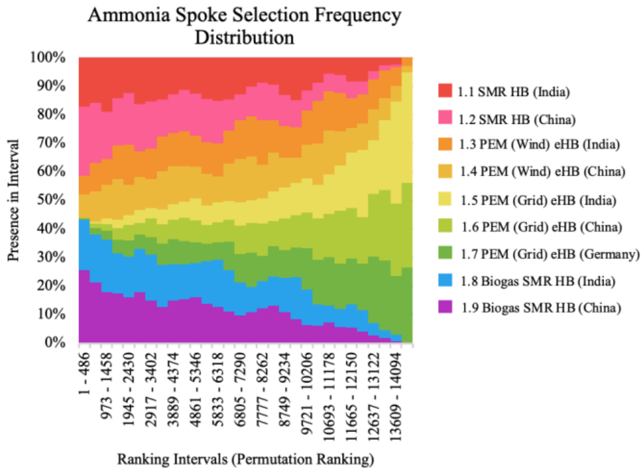
The Hou process based LCA results revealed though the earlier literature review (summarised in Table 6-5) showed a range of GWP indicator results between 1 tonne CO_2-eq per tonne soda ash to 2.2 tonne CO_2-eq per tonne soda ash. In comparison, the results from the hub and spoke's proof of concept show a GWP of 0.247 tonne CO_2-eq per tonne soda ash for the recommended value chain (permutation ID 14,439). This is clearly a significant difference. However, the LCAs in literature assume that all CO_2 feeds and energy demands are serviced through the combustion of coal. Contrasting this, the value chain recommended within this work utilises DAC for CO_2 feeds with energy supplied via biogas and hydroelectric sources. With this knowledge, it is unsurprising that GWP impacts are reduced, achieving a potential reduction of 75.3%. Given the screening nature of the proof-of-concept and its lack of sensitivity analysis, a smaller improvement may be realised if deployed in reality or studied with finer granularity. In addition, the literature assessments do not examine any other indicators, making it impossible to determine if this GWP improvement is achieved at the expense of other indicators (most likely economic based).

6.7.5.2 Examination of Spoke Selection Frequency Distributions

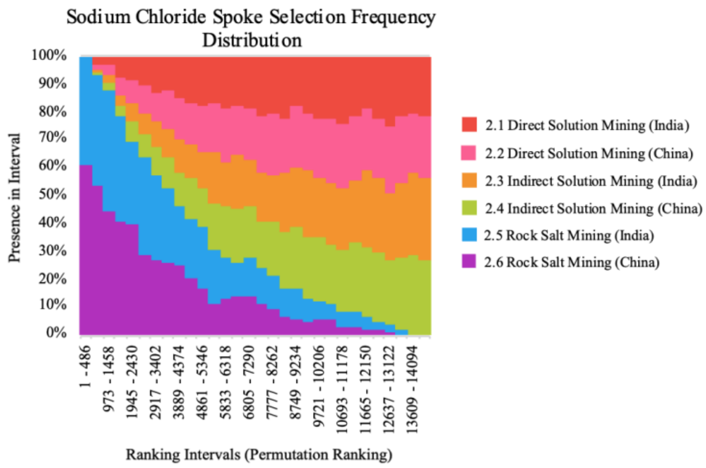
While the previous examination of the best performing hub and spoke permutations delivers significant utility to a FMCG company in the early stages of value chain development, additional information can be extracted by framing the generated data in a different way. To this end, frequency distributions are again utilised. However, this time, local spoke selection within each set is examined relative to global permutation rank. The spokes that are selected most commonly within the higher-ranking permutations are those that perform best within their local set. In addition to this, the magnitude and distribution of this frequency is indicative of the spoke sets influence on the overall value chain ranking. For example, if examining the top scoring 5% of value chain permutations, a spoke in set 1 present in 95% of scenarios wields more influence on overall performance than a spoke in set 2 that is present in only 65% of scenarios. Such a spoke selection frequency distribution therefore provides the FMCG company with twin insight generation;

1. Best performing spoke (considering the value choices specified through the AHP indicator weighting).
2. Relative influence of that spoke set on the overall value chain performance.

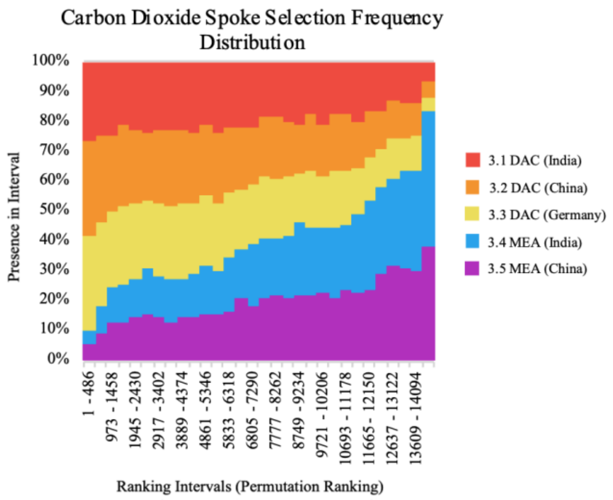
Applying this logic to the data generated in the proof-of-concept study, the 14,580 ranked value chains are split into 30 intervals, each containing 486 permutations. The selection rate of spokes within each interval is then evaluated, as a percentage, on a set-by-set basis. The results of this analysis are shown by Figure 6-32(a-e). Figure 6-33 through Figure 6-37 reformat this data to aid with interpretation by showing the most common spoke within each interval (sometimes ambiguous within Figure 6-32(a-e)).



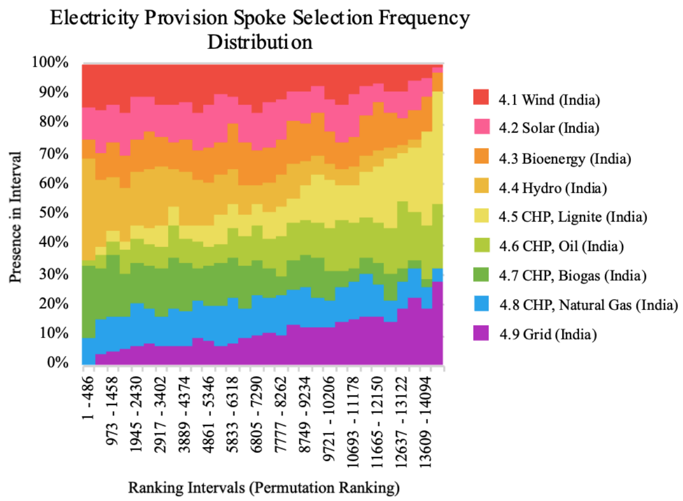
(a)



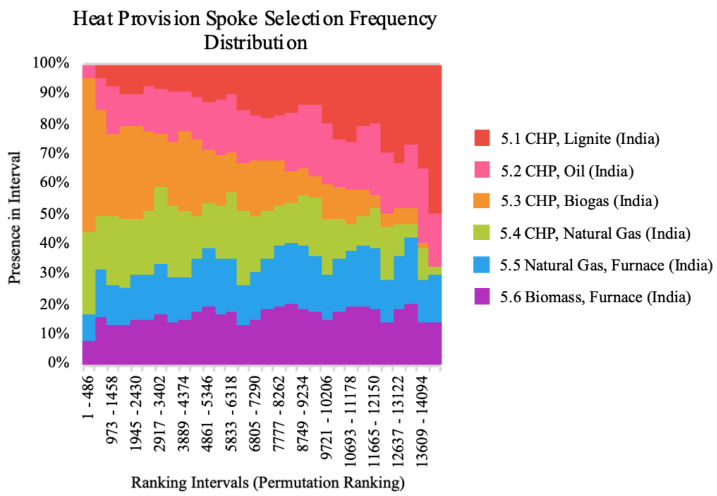
(b)



(c)



(d)



(e)

Figure 6-32(a-e) – Spoke selection frequency distributions relative to value chain permutation rankings.

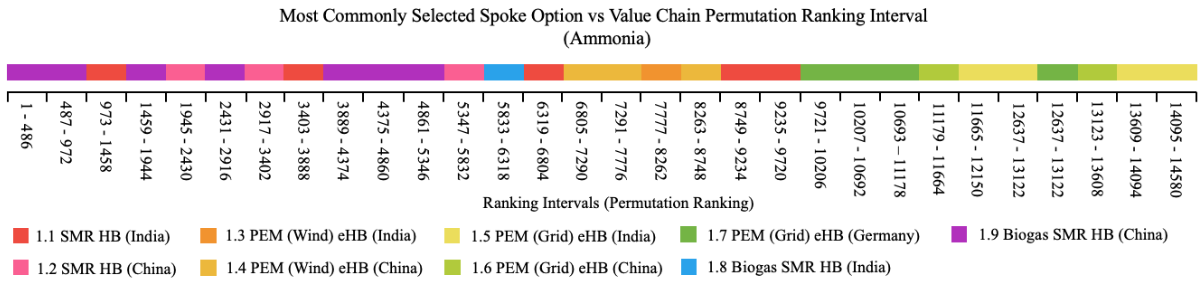


Figure 6-33 – Most commonly selected spokes from set 1 for each value chain ranking interval.

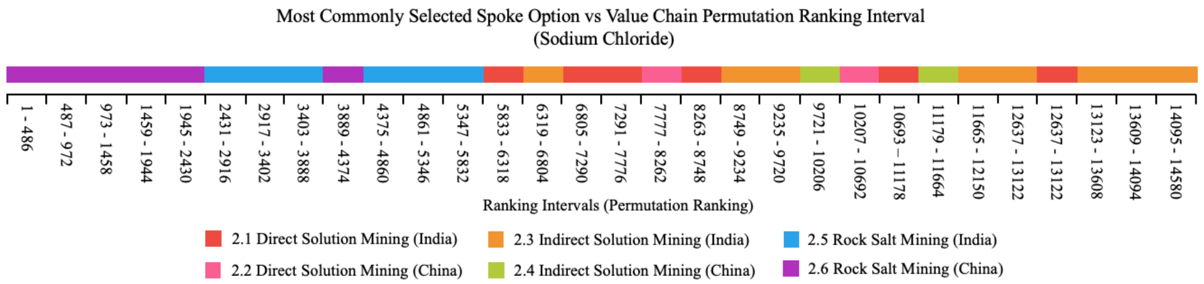


Figure 6-34 – Most commonly selected spokes from set 2 for each value chain ranking interval.

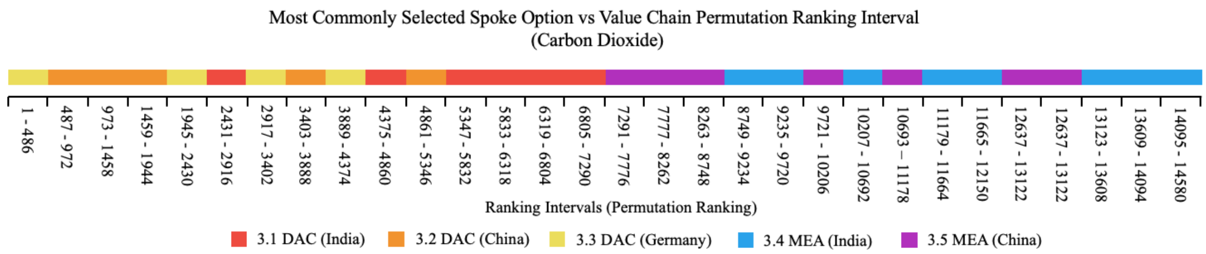


Figure 6-35 – Most commonly selected spokes from set 3 for each value chain ranking interval.

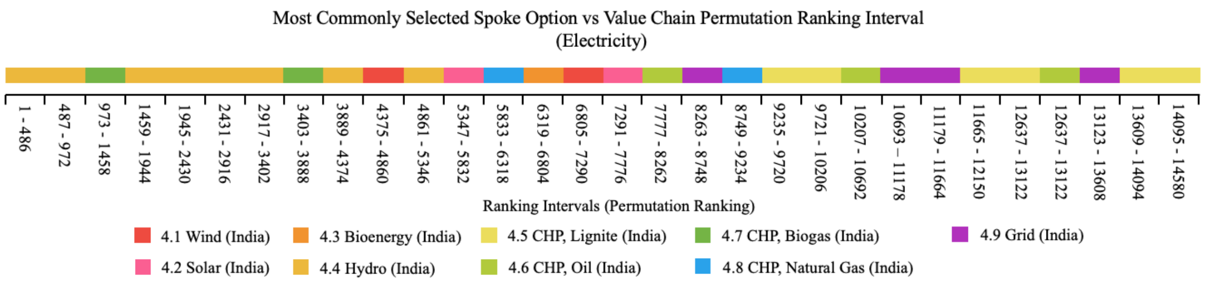


Figure 6-36 – Most commonly selected spokes from set 4 for each value chain ranking interval.

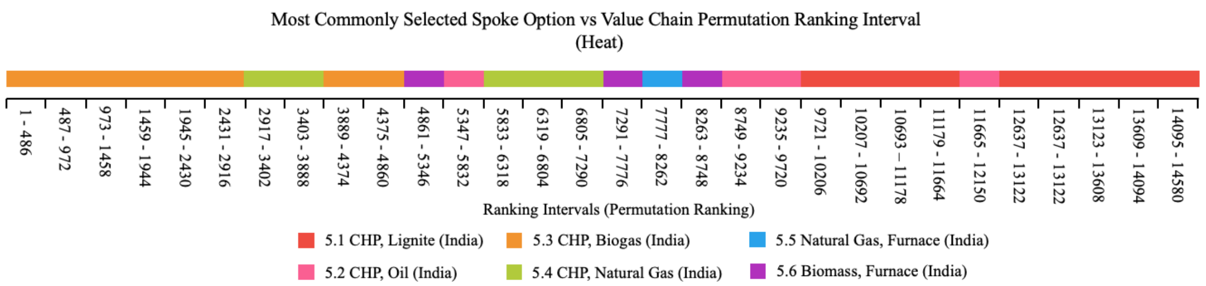


Figure 6-37 – Most commonly selected spokes from set 5 for each value chain ranking interval.

The figures prove highly effective in generating and communicating both of the insights noted above. For example, when consulting Figure 6-32b, it is immediately apparent that spoke 2.6 is the best performing within the set; a fact confirmed by Table 6-33 and Figure 6-27. Furthermore, the spoke's presence in 60% of value chains in the highest-ranking interval signals a significant advantage over the alternatives and notable influence on the overall value chains sustainability profile, mirrored by its uniform selection in Table 6-37.

As identified earlier, within the five best performing value chain permutations (Table 6-37), spoke selection from sets 2, 4, and 5 were uniform (I.D's 2.6, 4.4 and 5.3 respectively). When consulting Figure 6-32(b, d, and e) these spokes are indeed the most common selection in the highest-ranking intervals, confirming their dominant position as the best performing alternatives within their local sets. In fact, Figure 6-34 and Figure 6-37 show that spokes 2.6 and 5.3 respectively are the most common selection in all five of the highest-ranking intervals. Set 4, however, shows spoke 4.4 as the most common selection in only 4 of the first 5 intervals (Figure 6-36); with spoke 4.7 being the most common selection within interval 3 (permutation ranks 973-1458). This is explained by set 4 having the smallest score differential, and therefore certainty in performance advantage, between the best and second-best spoke (when considering only the sets with uniform selection across Table 6-37's five best performing value chains). This scoring proximity and associated uncertainty allows for the domination of spoke 4.7 within interval 3.

In contrast to these highly influential spoke selections, sets 1 and 3 exhibit much weaker selection trends. Considering first set 1, Figure 6-32a and Figure 6-33 visually indicate a very similar selection frequency for spokes 1.2 and 1.9 reflecting the very small difference of 0.009 between their respective subjective sustainability scores (as shown by Table 6-32). Set three is the only one to present three different spokes within the top five performing value chains, while also exhibiting the smallest range between best and second-best performing spokes at 0.004, and only 0.042 between the top three. Consequently, it can be said that spokes with similar selection frequencies within the best ranking value chain permutations do indeed have a similar subjective sustainability scores. This is reflected in Figure 6-32c, with the selection frequency of spokes 3.1, 3.2, and 3.3 being visually indistinguishable. Figure 6-35 notes spoke 3.3 as the most common selection within the first interval, this is indeed reflected in the set's constituent subjective sustainability scores within Table 6-34. However, interestingly, spoke 3.2 is identified as the most common selection within intervals 2 though 4, before interval 5 reverts to a modal selection of spoke 3.3. This is a clear example of a spoke set wielding little influence over the final value chain recommendation due to strong competition between its constituent spokes; in such scenarios the practitioner focussed objective assessment results should be consulted to evaluate trade-offs across specific indicators.

It was initially hypothesised that spoke sets containing larger numbers of competing alternatives would produce less easily interpretable selection frequency distributions; based on the assumption that less differentiation would be present within the constituent spokes' scores. However, once generated, the attained distributions disprove this assumption. For instance, spoke set 4, one of the most heavily contested with 9 competing alternatives, shows a clear selection preference for spoke 4.4. In fact, this proves easier to interpret visually than spoke set 3 (Figure 6-32c) with only 5 competing alternatives. Consequently, it can be concluded that interpretability of recommendations is dependent not on the number of constituent spokes, but rather the proximity of the most favourable options; a highly favourable outcome when considering both real world deployment and the FMCG specific needs outlined in Chapter 4.

6.7.5.3 Evaluation of Interpretation Techniques

Thus far, two philosophically different approaches to result presentation have been presented. Despite initially appearing to reiterate the same insights, the approaches are better viewed as two sides of the same proverbial coin. The first (Table 6-37 and Table 6-38) details the value chain structures for the five top performing permutations, examining the best performing alternatives under ‘high magnification’. The second (Figure 6-32(a-e) - Figure 6-37) more general approach examines the performance and selection behaviour of the spokes assessed within each set, offering a broader ‘low magnification’ view of the problem space.

Granular examination of the top performing value chain permutations provides clear and concise recommendations upon which decision makers and FMCG companies can mobilise. However, the reduction of such a large LCIA to five recommendations (out of 14,580 competing alternatives) represents a 99.97% data loss, inhibiting insight generation. In contrast, the examination of spoke selection frequency considers the full LCIA dataset, but in a lesser resolution. This allows for the identification of important spoke selections that are highly influential with respect to the overall value chain’s performance. Together, these approaches to analysis deliver a broad and functional understanding of the system and its potential range of impacts.

It is, for these reasons, proposed that the visual representations of spoke selection frequency offer significant value addition within the hub and spoke framework. Whereas quantified numerical LCIA results are of great value to a practitioner well versed in LCA, TEA and SIA, they are often of lesser value to the corporate or industrial decision makers who must act upon the assessment results in real terms. Communicability to a broad range of assessment stakeholders is a persistent stumbling block within sustainability assessment in general. The presentation of spoke selection and performance through Figure 6-32(a-e) - Figure 6-37 therefore provides non-technical stakeholders, such as FMCG decision makers, with more readily interpretable visual data upon which pragmatic industrial scale progress can be informed. Conclusions drawn from this data can then be buttressed by the parallel objective impact results as seen in Table 6-38.

6.7.5.4 Influence of Indicator Result Profiles on Permutation Ranking

A key component of the hub and spoke framework is the integration of decision maker value choices to deliver bespoke impact indicator weightings and tailored value cain recommendations. However, the use of uniform indicator weightings within the proof-of-concept largely nullifies the authority of these weightings, allowing for a deeper examination of factors exercising significant influence over the final value chain rankings. A primary driver for such non-MCDM derived ranking influence is the degree dispersion (standard deviation) observed within the 14,580 value chain permutations’ objective indicator results. It should logically be expected that indicators exhibiting a more diverse range of indicator scores, and therefore performance differentiation, should more strongly correlate with global permutation rank. CapEx is excluded in this analysis as it is only pertinent to the hub LCI as discussed in Chapter 4.

To examine this hypothesis, the overall objective indicator results are tabulated for all value chain permutations (in an extended form of Table 6-38). Each permutation is given local indicator performance rankings, assigning a rank of 1 to the best performing permutation in each indicator, and a rank of 14,580 to the worst. Given that the frameworks balances trade-offs across the 18 evaluated indicators in order to deliver recommendations, permutation's performance rankings within a specific indicator will not always reflect the overall, or global, ranking. The correlation coefficient observed between the local (indicator specific) and global rankings is then calculated independently for each indicator using Pearson's method [307] (results given in Table 6-39).

Having defined the degree of correlation between global and local permutations ranks, the standard deviations observed across each assessed indicator are evaluated. Due to the reporting of the value chains' objective impacts relative to locally defined units (e.g. kg CO_2-eq for GWP), the magnitude of the values varies between indicators, resulting in incomparable standard deviations. To resolve this 'apples vs oranges' comparability issue, the objective impact values are normalised across the 14,580 permutations for each indicator. This follows the same procedure used for the normalisation of intra-spoke-set indicator scores detailed in Section 6.7.2. Following this, dimensionless values between 0 and 1 are obtained (with higher values indicating desirable performance). Using this normalised data, the standard deviation observed across each indicator is evaluated. The resulting correlation between local and global permutation rankings, and each indicator's observed standard deviation, are given in Table 6-39.

Table 6-39 – Evaluation of global to local ranking correlation and observed standard deviation for each assessed indicator.

Correlation Between Standard Deviation of Normalised Global Objective Indicator Scores & Correlation to Value Chain Permutation Rankings																			
Statistical Test	Global Warming Potential (GWP 100)	Ozone Depletion	Metal Resource Depletion	Freshwater Eutrophication Potential	Marine Eutrophication Potential	Acidification Potential (Terrestrial)	Water Use	Energy Demand	Energy Efficiency	Mass Efficiency	OpEx/Procurement Price	Worker Health & Safety	Child Labour Risk	Forced Labour Risk	Utilisation of Hazardous Materials	Changes to Local Water Supply	Changes to Local Electricity Supply	Changes to Local Land Use	Correlation
Std Dev of Normalised Objective Indicator Results	0.2605	0.2521	0.3054	0.2812	0.2758	0.2793	0.2252	0.2413	0.0111	0.0357	0.1945	0.0222	0.0345	0.0254	0.0345	0.0464	0.0482	0.0340	0.8186
Global to Local Rank Correlation	0.7093	0.6983	0.5608	0.6921	0.7323	0.7018	0.7730	0.5902	-0.0203	0.5753	-0.0576	0.0237	0.0375	0.0299	0.0498	0.0545	0.0631	0.0686	

Table 6-40 - Evaluation of global to local ranking correlation and observed standard deviation for each assessed indicator (excluding mass efficiency and OpEx)

Correlation Between Standard Deviation of Normalised Global Objective Indicator Scores & Correlation to Value Chain Permutation Rankings																	
Statistical Test	Global Warming Potential (GWP 100)	Ozone Depletion	Metal Resource Depletion	Freshwater Eutrophication Potential	Marine Eutrophication Potential	Acidification Potential (Terrestrial)	Water Use	Energy Demand	Energy Efficiency	Worker Health & Safety	Child Labour Risk	Forced Labour Risk	Utilisation of Hazardous Materials	Changes to Local Water Supply	Changes to Local Electricity Supply	Changes to Local Land Use	Correlation
Std Dev of Normalised Objective Indicator Results	0.2605	0.2521	0.3054	0.2812	0.2758	0.2793	0.2252	0.2413	0.0111	0.0222	0.0345	0.0254	0.0345	0.0464	0.0482	0.0340	0.9696
Global to Local Rank Correlation	0.7093	0.6983	0.5608	0.6921	0.7323	0.7018	0.7730	0.5902	-0.0203	0.0237	0.0375	0.0299	0.0498	0.0545	0.0631	0.0686	

When examining the data in Table 6-39, a relatively strong correlation (*r* = 0.8186) is observed between the standard deviation of normalised objective indicator results and the alignment of local indicator and global permutation rankings. This strongly indicates that the previous hypothesis, that the primary driver for non-MCDM derived ranking influence is the degree dispersion observed within the objective indicator results, is correct. Furthermore, they exhibit a linear relationship. However, when plotted graphically in Figure 6-38, two notable outliers are present, the nature of which must be scrutinised and understood;

1. Mass Efficiency
2. OpEx / Procurement Price

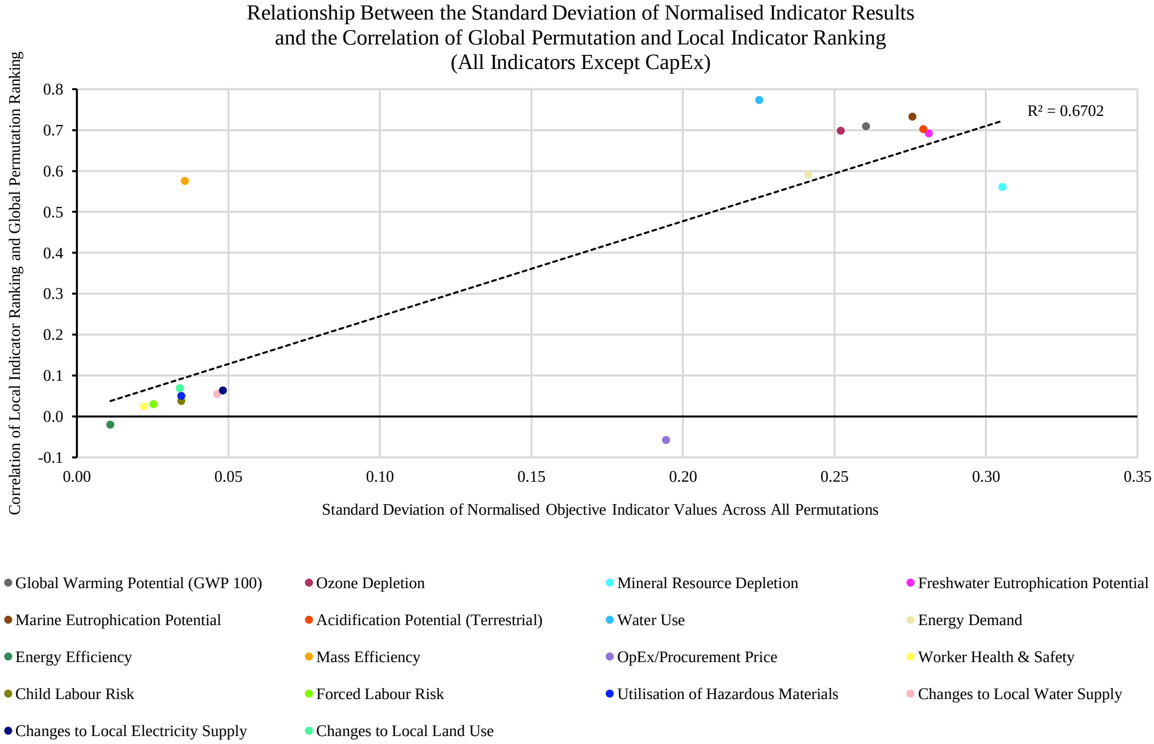


Figure 6-38 – Relationship between the standard deviation of normalised indicator result and the correlation of global permutation and local indicator ranking. All 18 indicators, excluding CapEx are included in respective data points.

Mass efficiency is the easiest of the pair to explain. As the mass efficiency indicator value falls, all other LCA and TEA indicators are negatively impacted (larger feedstock requirements, elevated OpEx, etc.), amplifying the effects via positive feedback. In this capacity, mass efficiency can be viewed as a loosely predictive factor for LCA performance. This explanation is supported by the moderately strong correlation observed between local indicator ranking and global permutation ranking (0.5753), despite having a low standard deviation with respect to the normalised objective indicator values (0.0357). This explanation is confirmed by examining the correlation between mass efficiency and other indicator's performances across the feedstock spokes. The results, shown in Table 6-41 indicate a strong correlation between spokes' mass efficiency performance and; ozone depletion, marine eutrophication potential, acidification potential and water use. Compounding this, only 2 of the 17 other indicators exhibit a negative correlation coefficient, both occurring within the social strand. As proposed previously, it is the LCA indicator performance that aligns with mass efficiency, with all social indicators exhibiting negligible correlations.

Table 6-41 - Correlation of mass efficiency performance to that of other assessed indicators for material spoke sets (excluding CapEx).

Indicator	Performance Correlation with Mass Eff.
Global Warming Potential (GWP 100)	0.2767
Ozone Depletion	0.7501
Metal Resource Depletion	0.5367
Freshwater Eutrophication Potential	0.4695
Marine Eutrophication Potential	0.7427
Acidification Potential (Terrestrial)	0.7440
Water Use	0.7205
Energy Demand	0.2551
Energy Efficiency	0.1687
OpEx/Procurement Price	0.1422
Worker Health & Safety	0.0259
Child Labour Risk	0.0307
Forced Labour Risk	0.0316
Utilisation of Hazardous Materials	-0.0309
Changes to Local Water Supply	0.0312
Changes to Local Electricity Supply	0.0055
Changes to Local Land Use	-0.0172

The second outlier (OpEx) arises through more convoluted causation, exhibiting the inverse behaviour to that observed for mass efficiency; possession of a notable standard deviation (0.1945) within the normalised objective results, but no observed correlation between local indicator performance ranking and global permutation ranking (-0.0576). Analysis indicates that spokes' OpEx indicator performance is being saturated out by moderately conflicting performance from other indicators; metal resource depletion, freshwater eutrophication potential, and energy efficiency. Compounding this, in many of the assessed spoke sets the estimated OpEx, or procurement price in the case of spokes, is inversely related to the performance observed within LCA indicators, the clearest example being the CO_2 feedstock routes (spoke set 3). The overall value chain performance corelations between OpEx and other indicators for feedstock spoke sets are shown below in Table 6-42. Generally, the strength of the correlations is much lesser than those observed for mass efficiency in Table 6-41, a fact that supports the proposed theory that the influence of OpEx is saturated out by the compounding performance of a majority of other indicators rather than strong opposition in a small number.

Table 6-42 – Correlation of OpEx performance to that of other assessed indicators for feedstock spoke sets (excluding CapEx).

Indicator	Performance Correlation with OpEx
Global Warming Potential (GWP 100)	0.3888
Ozone Depletion	-0.1123
Metal Resource Depletion	-0.3227
Freshwater Eutrophication Potential	-0.3645
Marine Eutrophication Potential	-0.1116
Acidification Potential (Terrestrial)	-0.0989
Water Use	-0.1464
Energy Demand	0.6858
Energy Efficiency	-0.4478
Mass Efficiency	0.1422
Worker Health & Safety	-0.1868
Child Labour Risk	-0.2644
Forced Labour Risk	-0.2615
Utilisation of Hazardous Materials	0.0334
Changes to Local Water Supply	-0.2077
Changes to Local Electricity Supply	-0.1292
Changes to Local Land Use	-0.0701

Removing these two outlying indicators (Table 6-40), the correlation between the standard deviation of an indicator's normalised objective values and the alignment of local indicator and global permutation ranking becomes much clearer (shown by Figure 6-39 below). The observed correlation coefficient also increases significantly, reaching a value of 0.9696, signalling the presence of a very strong correlation. Through this analysis it can be said that, generally, the standard deviation observed within indicator's normalised objective results is indicative of its influence on overall value chain rankings.

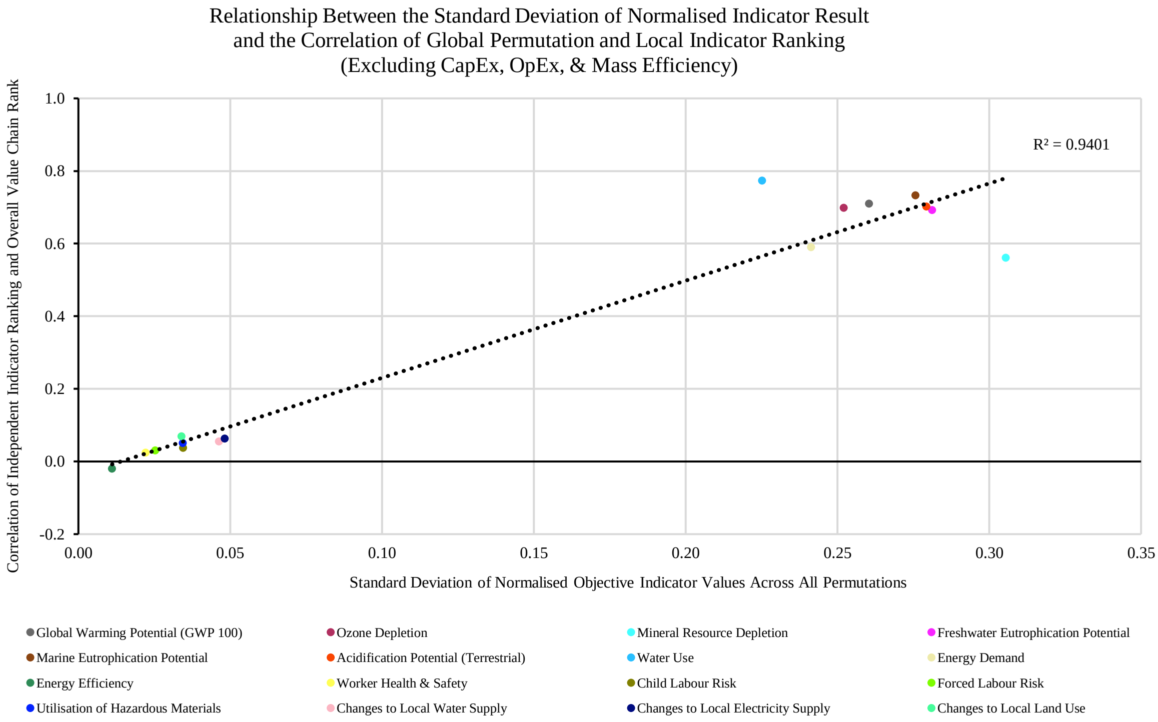


Figure 6-39 - Relationship between the standard deviation of normalised indicator result and the correlation of global permutation and local indicator ranking. All 18 indicators, excluding CapEx, mass efficiency, and OpEx are included in respective data points.

Overall, this analysis of the hub and spoke framework's performance indicates that the methodology is most effective when used in assessments evaluating indicators which exhibit performance differentials of comparable magnitude. In applications where objective results are tightly grouped within a specific indicator, it contributes little to the ranking of value chain permutations. However, this loss of authority is not necessarily associated with lacking framework efficacy. A low standard deviation in the normalised objective indicator results is suggestive of only a small real world performance differential. Consequently, it follows that the indicator should have less influence on final value chain recommendation than one with highly differentiated performances. In essence, a hypothetical 2% reduction in GWP should not logically be prioritised over a potential 50% reduction in ODP when it comes to calculating competing value chains' subjective sustainability scores (assuming roughly equal indicator magnitudes and weightings).

However, it must be noted that the hub and spoke framework's standard normalisation procedure does not account for scenarios where competing indicators possess objective results of vastly different magnitudes. Expanding upon the previous example, a 2% reduction of a 1000 kg-CO_2-eq / FU GWP value may, in real terms, outweigh a 50% reduction on an ODP of 0.1 kg CFC11-eq / FU. However, blind application the default max-zero normalisation would cause the framework to overlook this nuance, likely necessitating practitioner intervention. Recognition of scenarios such as this was a large driving factor for the parallel presentation of objective indicator results for each overall value chain permutation (as seen in Table 6-38). Through this, a deeper and contextualised appreciation of the indicator's magnitudes is attained. Remedial action from the practitioner would be justified in such eventualities. This could be achieved by either removing the ODP indicator due to the very small impact magnitudes, or, applying a utility curve or artificial normalisation bounds to reduce the influence of ODP on value chain recommendations.

6.7.6 Influence of MCDM Inputs

The final attribute of the hub and spoke framework requiring evaluation is the utility provided through, and influence wielded by, the MCDM (AHP) inputs. In essence, as a given indicators' AHP derived weighting increases, the correlation between permutations' overall ranking and their relative performance within that indicator should increase. To meaningfully examine this effect a systematic approach is necessary. This will examine the GWP of each assessed permutation and their respective recommendation ranking as the indicator's weighting is incrementally increase. GWP was selected for examination due to its relevance to the 'clean future initiative', a representative setting for the frameworks use, and the indicators position as the most commonly investigated LCA indicator (Figure 6-11).

For this inquiry, a set of eight weighting scenarios are defined by altering the AHP inputs to generate successively larger GWP weightings. The indicator weights obtained via these input scenarios are displayed in Table 6-43. As the scenarios progress the weighting assigned to GWP increases. In addition to these AHP input scenarios, a range of recommendation cut-offs are evaluated, considering the top 10, 25, 50, 100, 500, 1000, and 14,580 permutations respectively. This was deemed relevant as one of the framework's primary applications is the screening of all available feedstock suppliers followed by a recommendation of a small proportion of value chain permutations for more granular assessment.

Overall, the range of GWP indicator weightings evaluated was 0.05263 to 0.49091. The lowest of these values is representative of the equal indicator weighting scenario used in the previous sections, with the highest representing the maximum weight attainable through the tiered AHP structure (uniform score of 9 applied to the GWP and LCA rows seen in Figure 4-11). The permutations' GWP performance rankings were evaluated by assigning the value chain with the lowest emission value (per FU) a rank of 1, the second lowest a rank of 2, and so on. The correlation of this local indicator rank with the overall permutation rank was evaluated using Pearson's method [307]. The correlation strength between the GWP indicator and overall permutation ranks for the selected weighting scenarios and recommendation count cut-offs are displayed in Figure 6-40.

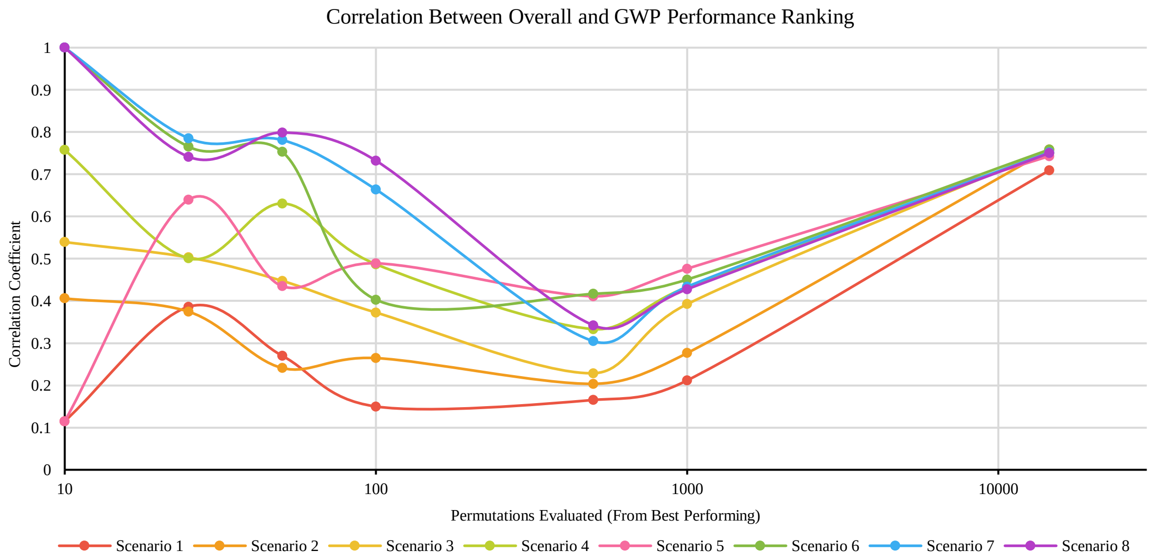


Figure 6-40 – The correlation observed between permutations relative GWP performance and the recommendation ranking. Scenarios reflect the indicator weightings shown in Table 6-43.

Table 6-43 - Indicator weighting scenarios used for the evaluation of MDCM inputs on value chain recommendations.

Indicator	Assessment Strand	Indicator Weights							
		Scenario 1	Scenario 2	Scenario 3	Scenario 4	Scenario 5	Scenario 6	Scenario 7	Scenario 8
Global Warming Potential (GWP 100)	LCA	**0.05263**	**0.12281**	**0.16746**	**0.19838**	**0.22105**	**0.36000**	**0.46667**	**0.49091**
Ozone Depletion		0.05263	0.04094	0.03349	0.02834	0.02456	0.04000	0.05185	0.05455
Mineral Resource Depletion		0.05263	0.04094	0.03349	0.02834	0.02456	0.04000	0.05185	0.05455
Freshwater Eutrophication Potential		0.05263	0.04094	0.03349	0.02834	0.02456	0.04000	0.05185	0.05455
Marine Eutrophication Potential		0.05263	0.04094	0.03349	0.02834	0.02456	0.04000	0.05185	0.05455
Acidification Potential (Terrestrial)		0.05263	0.04094	0.03349	0.02834	0.02456	0.04000	0.05185	0.05455
Water Use		0.05263	0.04094	0.03349	0.02834	0.02456	0.04000	0.05185	0.05455
Energy Demand	TEA	0.05263	0.05263	0.05263	0.05263	0.05263	0.04000	0.02222	0.01818
Energy Efficiency		0.05263	0.05263	0.05263	0.05263	0.05263	0.04000	0.02222	0.01818
Mass Efficiency		0.05263	0.05263	0.05263	0.05263	0.05263	0.04000	0.02222	0.01818
OpEx		0.05263	0.05263	0.05263	0.05263	0.05263	0.04000	0.02222	0.01818
CapEx		0.05263	0.05263	0.05263	0.05263	0.05263	0.04000	0.02222	0.01818
Worker Health & Safety	SIA	0.05263	0.05263	0.05263	0.05263	0.05263	0.02857	0.01587	0.01299
Child Labour Risk		0.05263	0.05263	0.05263	0.05263	0.05263	0.02857	0.01587	0.01299
Forced Labour Risk		0.05263	0.05263	0.05263	0.05263	0.05263	0.02857	0.01587	0.01299
Utilisation of Hazardous Materials		0.05263	0.05263	0.05263	0.05263	0.05263	0.02857	0.01587	0.01299
Changes to Local Water Supply		0.05263	0.05263	0.05263	0.05263	0.05263	0.02857	0.01587	0.01299
Changes to Local Electricity Supply		0.05263	0.05263	0.05263	0.05263	0.05263	0.02857	0.01587	0.01299
Changes to Local Land Use		0.05263	0.05263	0.05263	0.05263	0.05263	0.02857	0.01587	0.01299

General evaluation of Figure 6-40 shows that when considering the full count of 14,580 permutations, the correlations are of similar strength (0.709 – 0.759) for all weighting scenarios, indicating a consistently moderate to strong correlation. However, looking more closely at these correlation strengths, scenarios with lower GWP weightings appear closer to the bottom of the observed range, suggesting lower differentiation between alternative value chains overall scores. This behaviour generally continues through all examined recommendation count cut-off values.

When the larger recommendation count cut-offs are exercised (100, 500 and 1000), and the number of permutations included in the analysis is reduced (moving to towards the middle and middle left of Figure 6-40) and skewed towards the better performing value chain alternatives. As the cut-off count is reduced the weighting scenarios' correlation strengths diverge. Moving further, towards the smallest recommendation count cut-offs (10, 25, and 50), two groups of more interesting behavioural typologies are observed:

1. Convergent, and relatively stable, correlation behaviour for scenarios 6-8.
2. Divergent correlation behaviour, with significant instability, for scenarios 1-5.

These two behavioural typologies also align with the magnitude of GWP's indicator weight. The converging scenarios all exhibit weights ≥0.36, and those with divergent and erratic behaviour possess GWP weightings <0.23. To assist with deeper interpretation of Figure 6-40 the scoring profile for each scenario is plotted for all 14,580 ranked permutations (using the same approach as used in Figure 6-30), the results are shown Figure 6-41.

It is revealed through Figure 6-41 that the highly weighted scenarios (6, 7 and 8) that resulting in convergent correlation behaviour exhibit larger scoring ranges than the others. In turn, this delivers steeper gradients, and therefore greater differentials between successive value chain scores, causing stronger global (overall) and local (GWP) ranking correlations. From an alternate viewpoint, as the GWP weighting increases its proportional contribution to the value chain's overall subjective sustainability score grows; consequently, conflicting performances within other indicators are less capable of causing localised GWP rank reversals. It can therefore be said with confidence that at higher AHP weightings, an individual indicator's performance does in fact wield significantly more influence on the final value chain recommendation. Furthermore, as the FMCG company's inputs shift towards higher prioritisation of nominal performance in a given indicator, the certainty with which decision can be made increases; a consequence of the greater performance differential between the alternatives' overall subjective sustainability scores. Importantly, in the scenarios with GWP weightings ≥0.36, the local indicator and overall value chain rankings are perfectly correlated for the top 10 permutations, successfully delivering highly tailored recommendations based on the FMCG companies value choices.

Moving on to consider the scenarios within Figure 6-40 that align with behavioural typology 2, the overall scoring profiles seen in Figure 6-41 exhibit lesser gradients than the scenarios fitting typology 1. As previously noted, this has a significant effect on the differentiation between value chain alternative's scores. Therefore, the remaining indicators wield more relative power with respect to the overall sustainability score, often resulting in rank reversals within the indicator possessing only slightly elevated weighting (in this case GWP). Such rank reversals are also responsible for the erratic behaviour shown by scenarios 1-5 on the left-hand side of Figure 6-40, responsible for the out of sequence positioning of many GWP indicator performances.

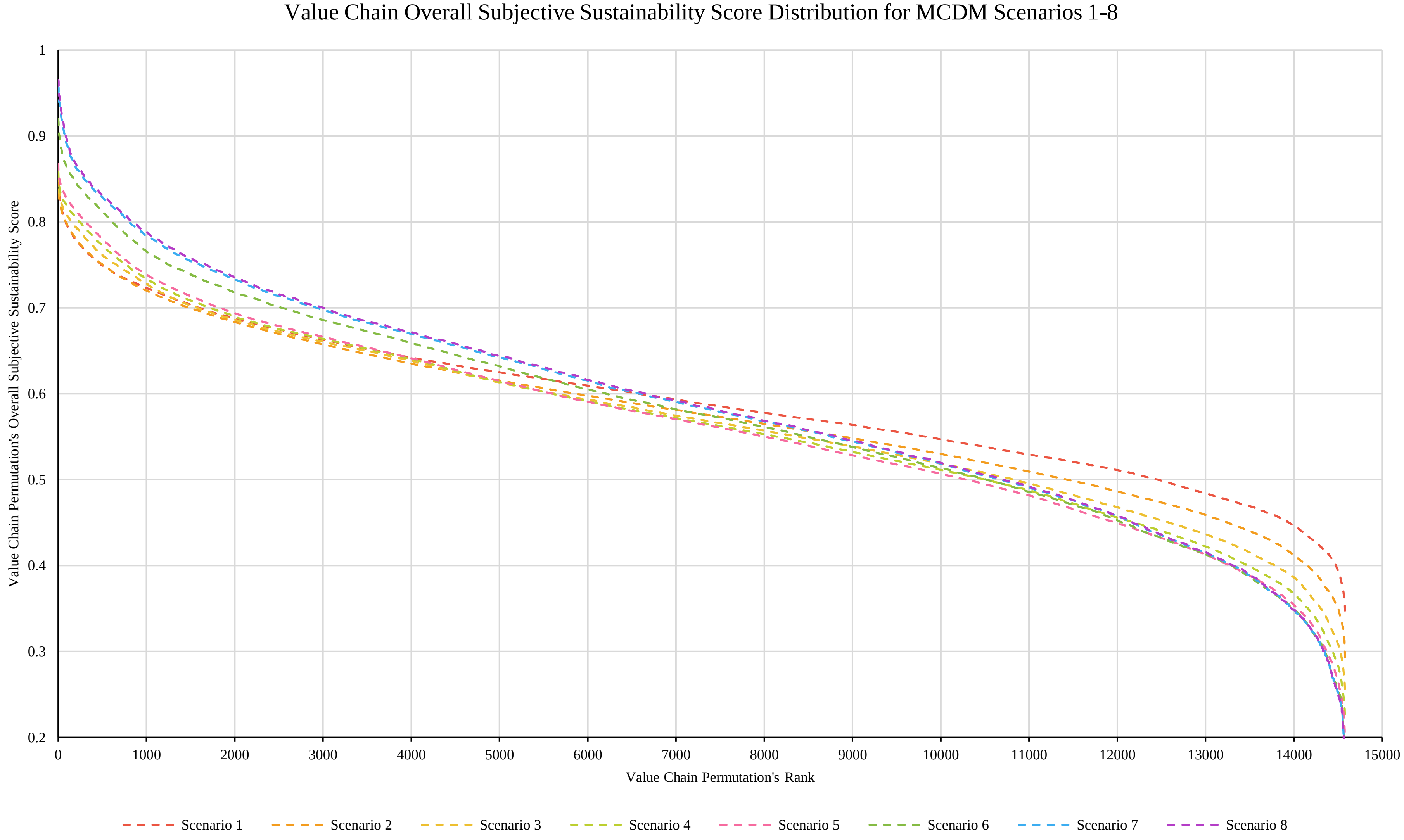


Figure 6-41 - Scoring profiles for MCDM scenarios 1-8.

Overall, the MCDM weightings are demonstrated to exercise appropriate influence on the final value chain recommendations presented by the hub and spoke framework. The identified susceptibility to rank reversal reflects the fact that only a slight weighting preference is prescribed for the GWP indicator, with the framework still very much acting to minimise impacts across the broader raft of indicators. In addition, this application of subjective value choices does not detract from the scientific value of the assessment as the objective indicator results of each permutation are presented in parallel. In real world applications this prevents organisations from misusing the tool to 'greenwash' corporate decisions. For instance, if their AHP inputs result in high weightings in OpEx and CapEx indicators, the high overall subjective performance scores will not disguise any potentially negative impacts in LCA or SIA indicators. During the transition towards sustainable industrial ecosystems, FMCG companies should be supported in pursuing performance improvements in a way that simultaneously assists their business, realising benefits for all stakeholders.

6.8 Critical Reflection on Proof-of-Concept Results

Given that this chapter aimed to evaluate the performance of the 'hub and spoke' framework, it was deemed appropriate to critically review its performance through the identification and discussion of revealed methodological blind spots. Several of the most pertinent and influential examples evading previous discussion are highlighted below, ranging from the completeness of LCI data, to market forces, and overarching LCA typology.

Firstly, it should be recognised that within this proof-of-concept study there are several LCI assumptions or omissions that influence the quantification of spoke impacts and their subsequent selection frequency distributions (Figure 6-32). Perhaps the most notable of these is the omission of transport impacts associated with spoke 3.3 – DAC (Germany). If CO_2 was shipped between the two countries on a LNG vessel, the unidirectional trip distance is approximately 7,450km (4,630 statute miles) based on 2023 shipping corridors between Hamburg and Mumbai [308]. This maritime leg alone (sans land based rail or road legs) would be responsible for a GWP contribution of 50 kg CO_2-eq. [72], reducing the benefits of the CDU by a great enough magnitude to cause a rank reversal between permutation 14,439 and 14,385 in Table 6-38. This verifies that transport can be a significant contributor to impacts, constituting 16.8% of total GWP for permutation 14,439 (best performing alternative). Consequently, in any full assessment for the development of global value chains, transport must be carefully considered.

In addition to the aforementioned transport considerations, the framework fails to consider the available capacity of each feedstock production route. Within the proof-of-concept study this would likely to be relevant in the case of Biogas, utilised in spokes 1.8 – Biogas SMR HB (India) and 1.9 – Biogas SMR HB (China). With the six greatest producing countries generating 244 TWh of biogas per year [309], available capacity is significantly smaller than competing feedstocks such as natural gas (44,310 TWh per year) [310]. Given this disparity in global production capacity, the effects of competition for biogas as a electricity, fuel and biochemical feedstock should be incorporated in order to deliver a fair comparison between alternatives. The impacts of competitive markets are most likely to be observed within the market price of the affected commodity (TEA), or resource scarcity (LCA). Where this issue is expected to arrive, a sensitivity analysis should be conducted to consider the effect of elevated purchase prices on value chain recommendations.

Finally, the framework provides a methodologically rigorous tool for holistic FMCG sustainability assessments via an attributional rather than a consequential approach. The core difference between attributional and consequential assessment typologies is found in their philosophical approach to system boundary specification (shown visually in Figure 6-42). Attributional assessments follow a descriptive philosophy, aiming to allocate and quantify the inherent burdens of a product or system as it operates, using (typically) average data and fixed assessment boundaries. It is well-suited for benchmarking and corporate reporting. Contrasting this, consequential assessments adopt a predictive philosophy, focusing on how a decision changes the overall system, inclusive of market shifts, supply chain reactions, and other indirect effects. It seeks to model cause-and-effect relationships and is better suited for policy analysis and long-term strategic planning.

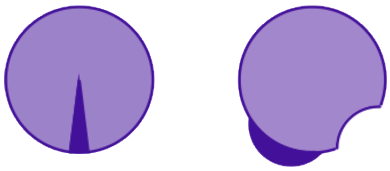


Figure 6-42 – Visual representation of attributional and consequential assessment types.

Within the 'hub and spoke' framework an attributional was selected owing to its consistency, comparability, and practitioner accessibility. Furthermore, its selection was deemed necessary to achieve the desired modular and interoperable LCI structure, a significant valorising factor within FMCG applications (as discussed in Chapter 4), achieved through the alignment of LCA, TEA and SIA system boundaries at both the spoke set and overall system levels. However, the approach introduces limitations when applied to decision-making in complex and evolving supply chains such as those found in the FMCG sector.

The attributional approach constrains the framework's ability to inform on market-mediated effects, co-product impact allocation, and ability to capture the broader systemic consequences of industrial decision-making. A relevant example can be drawn from the biogas discussion earlier in this section. Within a consequential assessment the limited production capacity relative to other assessed alternatives would be highlighted, making it significantly more likely that practitioners and decision makers would account for competitive procurement and pricing, or need for a diversified feedstock portfolio. Allocation of impacts to co-products can also be handled more representatively via consequential assessment. Attributional assessments typically assign a portion of a system's impacts to each product and co-product, often on a mass or economic basis. This is recognised as an imperfect approach that imposes arbitrary system-external rules rather than reflecting actual cause-and-effect relationships. Consequential assessments generally avoid allocation issues entirely by using system expansion or substitution. This credits the assessed system with the avoided impact from a co-products alternate production route, ensuring that impact burdens are assigned based on real-world cause-and-effect dynamics rather than arbitrary partitioning.

Clearly, the consequential approach's ability to estimate the reactionary system-wide implications of a decision would remedy many of the issues associated with attributional assessments, offering highly valuable and long term insights. However, this benefit would be delivered at the expense of workload and complexity. Within an attributional assessment system boundaries are often difficult to harmonise across a spoke set, this task becomes much less approachable when adopting a consequential philosophy. Such failure to accurately align system boundaries at the framework's spoke set and value chain level could render any results or comparative assertions useless. Consequently, given the aims and objectives of the 'hub and spoke' framework, an attributional approach was deemed the most appropriate option, with the caveat that limitations around potential market effects and impact allocation are clearly communicated during the interpretation phase.

6.9 Conclusion

This chapter set out to apply the FMCG and CDU oriented hub and spoke framework, and impact pathway-oriented SIA characterisation models, developed within Chapters 4 and 5 respectively. The resulting proof-of-concept study was oriented around the production of soda ash within the APAC region, and more specifically India. This scenario was selected due to production scales (65,940,000 tonnes in 2024) and the fact that it is highly representative of the sustainability insights desired by FMCG companies. Moreover, soda ash production is hard to abate with respect to GWP, typically relying on classical long standing value chains. Consequently, a new and holistic approach that broadly examines the cradle-to-gate sustainability profile of its production is both novel and of notable value to a FMCG company.

A review of literature was conducted to identify and characterise the main production routes; identified as the Solvay, Modified Solvay, and Hou processes. Having summarised the reaction steps and feedstock requirements for each, it was necessary to identify a single process upon which the proof-of-concept study would focus. To inform this selection initial mass balances were developed for each process and the potential for CDU integration evaluated. Through this, the Hou process was identified as the best suiter for a full assessment owing to two key factors (originally outlined in Table 6-11);

1. Largest baseline CO_2 uptake potential (at 100% reaction step conversion efficiency)
2. Largest proportion of reaction step capable of CO_2 uptake

In addition to this review of production routes, a systematic literature search was conducted to identify existing sustainability assessments that focus on soda ash production. Overall, the literature was sparse, offering only five publications focussing on the three identified processes. Furthermore, these were highly opaque, offering no insights into the LCI data, and in some cases not outlining a system boundary at all. In addition, it was noted that all CDU integration efforts around soda ash production have focussed on downstream waste products and their CO_2 mineralisation potential, neglecting CDU opportunities within the production itself and upstream value chain.

A comprehensive range of indicators were evaluated within the proof-of-concept study, delivering a broad understanding of value chains' sustainability profiles and spanning a wide range of data availability scenarios. For LCA, the most developed and standardised strand, the selection of both indicators their characterisation methods were based on usage frequency in literature. This approach was chosen to demonstrate the high degree of comparability that is attainable between the hub and spoke framework and more traditional LCA specific assessment methodologies. TEA indicators and characterisation methods were selected to provide utility to FMCG companies. An economic evaluation of the hub process' equipment purchase and installation costs are therefore included, as well as OpEx estimates based on price estimates for spoke inputs; these approaches were selected to reflect the organisations sphere of influence and financial accountabilities. Finally, the SIA strand deploys the indicators and characterisation methods developed in Chapter 5, exercising the methodologies and verifying their projected utility.

Having identified the Hou process as the hub process for the proof-of-concept, spokes were selected to provide a set of representative feedstock routes with suitable TRLs for immediate or near-future deployment. This encompassed the provision of; sodium brine (NaCl), ammonia (NH_3), carbon dioxide (CO_2), electricity, and heat. A total of 35 spokes were evaluated across these five sets. LCIs were subsequently generated for the hub and spokes. These were underpinned by mass balances, Ecoinvent v3.8, and literature data. The results were generated using Excel and recorded in the standardised datasheets developed in Chapter 4, verifying their capability and fitness for purpose. Each of these LCI datasheets can be found in Appendix C, with a demonstrative set of spokes generated for national level grid electricity production (Section 6.6.3.1).

The LCI/LCIA phase was carried out in two distinct parts: the independent consideration of spokes within their constituent sets, and the evaluation of fully aggregated value chain structures. Within the proof-of-concept study the subjective MCDM derived results were calculated using uniform indicator weights, providing the most balanced and representative overview of framework performance. The aggregation of the hub and spokes delivered a total of 14,580 unique value chain permutations for full assessment. Simultaneous calculation of every permutation's objective and subjective impact results robustly demonstrated the efficiency of the hub and spoke framework, evaluating in seconds what would otherwise take vast lengths of time if examined independently.

The results and discussion initially focussed on the framework's scoring of the 35 independent spokes and 14,580 overall value chain permutations. Evaluation of the spoke LCI/LCIAs on a local basis verified that the delivered results were logical and adhered to the field's general consensus. Furthermore, it demonstrated that the technologies and feedstock routes selected for inclusion exhibited both highly competitive alternatives, and options with significantly differentiated performance profiles across the impact indicators. Overall, this provided a situationally complete set of data upon which to test the aggregation procedures.

Having theoretically calculated the workload reduction associated with the utilisation of tiered AHP in Chapter 4, a maximum time saving of 68.63% in nominal conditions was indicated. When evaluated within the proof-of-concept study, providing a comparison under real life conditions, a 67.84% reduction in required pairwise comparisons was realised; this small divergence is attributable to non-uniform indicator distribution across the three strands.

Through application of the novel SIA characterisation models, developed in Chapter 5, a key avenue for future development is revealed. In applications such as this proof-of-concept, the national level resolution of the social impact risk provides a less than ideal performance range from which to distinguish feedstock sources. The co-examination of Indian and Chinese feedstock sourcing did allow the characterisation methods to deliver a measurable degree of differentiation; however, a second iteration of the methodologies including sector or material specific adjustment factors would add significant capability.

Once the 14,580 value chain permutations had been evaluated, and their impacts quantified, the overall scoring profile was examined. This revealed an approximately normal distribution, characterised within Figure 6-30 and Figure 6-31. The range, standard deviation, and mean of the scoring distribution were then evaluated. A range of 0.501 (>50% of that mathematically possible) and standard deviation of 0.088 indicated that the framework's results normalisation process is highly capable of generating well dispersed ranges of overall subjective sustainability scores, from which industrially relevant conclusions can be easily drawn. In addition, the mean of 0.588 indicates that the procedures are effective at centralising the average performance within the scoring range (0-1). The relatively fine 'tails' mean that value chain permutations with promising performance can be easily extracted from the overall set through the application of recommendation cut-off criteria (e.g. alternatives with overall subjective sustainability scores $> \mu + 2\sigma$).

For the proof-of-concept the value chain recommendations were delivered through presentation of the top five performing alternatives (permutations I.D.s 14439, 14385, 3099, 3045, and 14331 respectively). These strongly suggest that soda ash production in India should utilise; ammonia from biogas SMR in China, sodium chloride from rock salt mining in China, carbon dioxide from DAC, hydroelectricity from India, and the purchase of heat from local CHP facilities. However, a second, potentially more insightful approach to the presentation of results was developed by graphically examining the frequency distribution of each spoke's selection from their local set; revealing their relative influence on the overall value chain scores. Presentation of the recommendations in both formats provides a level of analysis unattainable through other methodologies.

Due to the fact that there are no comprehensive LCA, TEA of SIA studies of the Hou process or its extended value chain available in the literature (as detailed in Section 6.3.2 and Table 6-5), the results generated by the model can only be compared to the corresponding Ecoinvent 3.8 data. The only available data set is based on estimated global averages and utilises the most common feedstock production routes. However, when evaluated using the same allocation procedures and system boundaries, the delivered impacts are remarkably similar to those of the hub and spoke framework. To provide as fair of a comparison as possible to the global average used within the Ecoinvent data, a mean of the hub and spoke models GWP values will be used (spanning all 14,580 value chain permutations). This average returns a value of 2.77 tonnes CO_2-eq. per tonne soda ash. In contrast, the Ecoinvent data presents a value of 2.79 tonnes CO_2-eq. per tonne soda ash; delivering only a 0.717% difference between values. It must be noted that this validation should be accepted with caution as it requires the underlying assumption that Ecoinvent's global mix of feedstock provision matches the routes assessed within this research. Nonetheless, it is deemed reasonable to use this as evidence of an accurate hub and spoke LCI aggregation procedure.

The second half of the results and discussion focuses on understanding and verifying the mechanistic functionality of the framework. This brought to light many unplanned but useful aspects of the methodology and underpinning mathematics. A key example of this is the revelation and verification that the standard deviation observed in each indicator’s results across all value chain permutations is a strong predictor of it’s influence on value chain recommendations and overall subjective sustainability scores. Once identified, this is a logical conclusion. However, its apparency in the generated results goes a long way to validate the hub and spoke framework’s handling of performance trade-offs.

It was also demonstrated that, in some cases, this standard deviation-based prediction of indicator influence is not a concrete rule; two outliers were identified. These demonstrated that overarching correlations between sets of indicators (typically within the LCA strand) can artificially saturate out the effect of conflicting performance in a single other indicator that possesses a large standard deviation of results (OpEx exhibited this behaviour within the proof-of-concept). Although interestingly, a hypothesis stated in Chapter 4 was proven partially correct. It was suggested that OpEx and GWP are negatively correlated, this was proven via a realised magnitude -0.4.

Finally, the effect of AHP derived MCDM weightings on the value chain recommendations was examined. In this, the weighting of GWP was altered systematically, delivering eight unique assessment scenarios. Evaluation of performance across the scenarios showed that the base case utilised for the main results section, using uniform indicator weightings, was the least effective configuration for differentiating between the alternative’s overall performances. As the weighting distribution becomes less uniform, the scoring differential between the value chain permutations increases, therefore aiding selection. Having positively evaluated the hub and spoke framework’s performance in its least efficacious configuration, it can be said with confidence that the integration of the MCDM techniques has added significant value to industrial sustainability assessments.

Overall, it has been demonstrated that a highly effective and methodologically valorising framework has been developed. Through its modular structure it is more efficient than preceding approaches. Meanwhile, the parallel integration of MCDM to provide tailored and actionable recommendations allows organisations to measure the alignment of process routes or suppliers with their own corporate strategy. It is hoped that this work proves that such corporate strategy does not have to exist in conflict with sustainable development. Rather, they can both realise benefits though symbiotic development.

7 Conclusion & Future Work

7.1 Conclusion

With average atmospheric CO_2 concentrations surpassing 420 ppm, broadly increasing scepticism around attainment of the Paris Agreement targets, and increasingly divided societies, efficacious sustainability assessments have never been so relevant. Reflecting this, the overarching narrative of this thesis can be viewed as a philosophical exploration of one broad, yet immeasurably consequential, question.

How can sustainability assessment, at both the theoretical and methodological level, support the FMCG industry's progress towards holistically sustainable value chains, while simultaneously minimising negative impacts on the business models that facilitate the development of next generation solutions?

While a pragmatic and objective reader will identify nothing controversial within this statement, today's socio-economic climate has cultivated a hot bed of politicised attitudes regarding the effectiveness and transparency of industrial sustainability initiatives. On one hand, unconstrained capitalistic greed has periodically resulted in the side-lining of environmental and social issues, exemplified by DuPont's legally negligent and highly impactful release of methyl mercaptan in 2014 [311]. Conversely, deliberately disruptive, inflammatory, and socially divisive protests weaken public support for, and industrial ability to fund, research towards sustainable industrial ecosystems [312]. As with all complex systems, sustainable and equitable modern societies will not be realised through the manipulation of a single lever; rather, it requires the coordinated and complimentary action of all actors.

In cognition of this fact, industry must vigorously pursue improvement across their sustainability profiles. This must in turn be supported by researcher's development of methodologies that efficiently, quantifiably, and repeatably guide this progression; all while balancing trade-offs between environmental, economic, and societal factors. Such needs have been recognised within the concept of 'the triple bottom line' for three decades; being conceived in 1994 by business writer John Elkington. However, as proven through this thesis' literature review, the field of sustainability has been slow to develop effective methodologies that holistically evaluate process or value chain performance across all three strands. Consideration of each aspect in isolation prevents the identification of burden shifting between impact compartments; a fact highlighted by the case study in Chapter 3 that examines social inequalities arising from the adoption of EVs.

The work contained within this thesis aimed to further harmonise the environmental, economic and societal assessment strands in support of Unilever's Clean Future initiative. To this end, Chapter 3 delivered a literature review within which four major objectives were tackled. Objective 1.1, determination of the CDU oriented state of the art within each assessment strand, revealed these to be; the ISO 14040 standards and GCI guidelines for LCA, the GCI guidelines for TEA and the triple helix framework within SIA. Following this, and addressing Objective 1.2, the degree of methodological alignment was systematically examined. Findings show that the ISO 14040 standards act as a backbone within harmonisation efforts. In terms of goal and scope setting, the aforementioned CDU relevant practitioner guidance documents show 78% and 89% ISO alignment for TEA and SIA respectively. However, the available impact characterisation methods within SIA deviate significantly from its LCA and TEA counterparts. Utilising the findings of the literature review, a novel taxonomy of CDU applicable guidance was developed (Figure 3-9), confirming the triple helix framework as the only holistic approach to sustainability assessment within the CDU sub-field (Objective 1.3). This facilitated the pinpointing of prominent gaps in capability (Objective 1.4) for rectification. Of these, the most significant were the development of impact pathway SIA characterisation methods to eliminate the subjectivity of practitioner led reference scale alternatives, comparability issues arising from the development of intraoperable methodologies in favour of interoperability, and the identification or development of TEA and SIA databases to fill the role of LCA's Ecoinvent.

Following this scoping exercise, the thesis' primary objective of methodological development was approached. Given that ISO 14040 underpins a majority of post 2006 assessment guidelines, alignment to its methodology is baked into the guiding philosophy (Objective 2.1). This decision ensured adherence to the values of the field while also delivering interoperability and a future-proofed foundation. Consequently, the parallel evaluation of the assessment strands through ISO's four-phase format was deemed essential, allowing for meaningful bottom-up integration and inter-strand cross-linkages during both LCI and interpretation phases. Additionally, the uniform adoption of quantified and repeatable impact characterisation methods is mandated, avoiding utilisation of the SIA approach deployed within the Triple Helix. The final major requirement was the prevention of methodological interference from the inclusion of MCDM to support repeatable decision making. Therefore, any application of MCDM must be emancipated from the data flow through which robust objective indicator results are derived at the earliest opportunity.

Subsequently, to ensure that key methodological decisions were fit for application within the setting of FMCG value chain decision making (Objective 2.2), literature was consulted in the form of market and consultant led strategy reports. This revealed the industry's call for a focus on incorporation of the following capabilities: identification of partnership opportunities, generation of data to monitor progression in sustainability profiles, integration of corporate strategy and sustainability, communicability of sustainability performance to non-practitioners, and a focus on affecting change in the areas over which the company wields the most influence.

The establishment of these principles and requirements is apparent throughout the framework's entire architecture. At its core sits a hub and spoke network topology, incorporated in order to easily and simultaneously evaluate a plethora of potential partner organisations or process routes across a variety of required feedstocks and utilities. Deployed in applications ranging from commercial aviation route development to cloud computing, its selection was approached through a review of required characteristics and available techniques. These specified characteristics were based on the current constraining factors within FMCG LCAs and targeted; the ability to comparatively assess a high number of permutations, integration of MCDM to repeatably balance trade-offs across many indicators, and the ability to conduct either comprehensive or screening assessments. In this configuration, hubs represent process(es) under the commissioning organisation's influence, and sets of spokes represent procurement options for each of the hub's boundary flows (feedstocks and or wastes). Through this approach, the hub and spoke framework's LCIs adhere to Ecoinvent's homologation of impact reporting to a reference product; however, it also builds upon this approach to include the TEA and SIA indicator results. The selection of this topology results in a framework that is, in theory, infinitely expandable. Additionally, this approach results in more efficient subsequent assessments. Where the same feedstock material is required for a different hub process and assessment, the relevant spoke set LCIs can be directly transposed (provided comparable purity requirements and geographical constraints).

This interoperability of hub and spoke LCIs between assessments was key in attaining Objective 2.4. Detailed in Appendix B, standard data sheets were developed, providing practitioners with a template that specifies the data required for operability within the framework. These data sheets also contain and clearly display important information pertinent to the determination of the LCI's representativeness within secondary assessments, safeguarding against improper propagation.

As established, the goal of systematically harmonising the three assessment strands for industrial decision making presented an ideal opportunity for the integration of MCDM within the framework (Objective 2.3). The potential presence of many impact indicators, and the aim of selecting a value chain from very large numbers of competing alternatives, make MCDM a powerful tool if integrated meaningfully. It allows, for the first time, a truly repeatable and robust way to manage burden shifting. While MCDM is a contentious topic within pockets of the sustainability assessment community, owing to its inherent subjectivity and reduction in results granularity, this work circumnavigated these shortcomings via the two-pronged reporting strategy mandated within the guiding philosophy. In addition, sceptical practitioners are correct to point out that the objective performances of different sustainability impact indicators are not directly comparable, a pre-requisite for MCDM deployment. For this reason, in parallel to the traditional objective results, normalised values are generated within each spoke set and indicator, delivering relative and levelized scores. Procedures for normalisation are at the practitioner's discretion, however, a max-zero approach is suggested as standard practice. These normalised results, along with AHP derived indicator weightings form the basis for TOPSIS led value chain permutation scoring and ranking. Crucially, the isolation of the two reporting streams nullifies the well-founded trepidation associated with MDCM and indicator aggregation. The selection of a hybrid AHP-TOPSIS MCDM approach was supported by a review of 72 previous LCA applications (utilising 13 different methods) and seven FMCG relevant utility criteria. Furthermore, specification of a tiered AHP component realises a >68% reduction in workload. In the case of an assessment examining 18 impact indicators, the number of pairwise comparisons required falls from 153 in a global configuration to 48 in a tiered configuration. This saving is of value in all assessment applications but is further valorised in FMCG applications, requiring rapid decision making while considering large numbers of variables. The outlined developmental efforts result in a complete and functional framework architecture, realising the final objective (2.5) of Chapter 4.

With a suitable network structure, methodological architecture, and MCDM approach, the harmonisation of strand's impact characterisation methods was required (as determined in Chapter 3). Up to and including McCord *et al*.'s Triple Helix framework, SIA exhibited a significant and field wide gap in both knowledge and capability regarding impact characterisation. Where LCA and TEA deploy quantitative and broadly adopted characterisation methods, SIA is significantly less developed. A brief review of current characterisation options (Objective 3.1) revealed that existing social assessments typically utilise far less repeatable and objective reference scale approaches; relying on practitioner led scoring against (often fuzzy) criteria. To remedy this and deliver characterisation models compatible with the hub and spoke framework, Chapter 5 charts the development of LCA aligned impact pathway SIA characterisation models.

High quality and voluminous data sets underpin all good characterisation models, a fact recognised and reflected through Objective 3.2. The World Bank database was identified as the best suitor for this role within the SIA strand. The seven indicators evaluated were selected based on relevance to CDU (and therefore Unilever's Clean Future initiative) and represent a first of their kind approach. To attain the targeted national level scoring granularity, both a novel philosophical approach and a vast amount of data were necessary. Development efforts resulted in full coverage for a total of 129 countries and partial coverage across a further 110, fulfilling Objective 3.3. With these impact pathway-based characterisation models, the hub and spoke framework reaches a previously unrealised degree of methodological harmonisation across the three assessment strands.

Given the national level resolution of the developed models, their applications are clearly limited. The list of ideal applications includes but is not limited to; explorative assessments of future supply chains (inherently lacking in geographic specificity), screening assessments in which only a red-flag approach is required, or assessments of opaque value chains for which more granular data is not available. Despite this notable restriction on applicable use cases, the ability to repeatably and quantitatively evaluate the risk of social impacts along the full length of a complex FMCG value chain closes a significant gap in assessment capability.

With the incorporation of these two novel contributions, the framework architecture and SIA characterisation models, this research removes several persistent barriers to the conduction of meaningful holistic sustainability assessments. However, to verify the efficacy of the overall methodology, a proof-of-concept study was required. This was approached through a cradle-to-gate assessment of potential soda ash value chains in the APAC region. As a significant contributor to emissions within Unilever's procurement portfolio, improvements within soda ash value chains have the potential to move the needle on the business' overall sustainability profile. In addition to this, and recognising purple carbon within the Clean Future initiative, the study targeted the use of purple (CO_2 derived) carbon feedstocks.

With the product and functional unit (1 tonne of soda ash) specified, selection of a hub process was required. The three most capacious synthetic production routes (Solvay, Modified Solvay, and Hou) were therefore evaluated, aiming to determine their inherent CDU potential (Objective 4.1). As the best performer in all examined criteria, the Hou process was adopted as the hub (Objective 4.2). In order to service this hub with feedstocks, the following five spoke sets were populated;

1. Ammonia
2. Sodium chloride brine
3. Carbon dioxide
4. Electricity
5. Heat

In total, 35 independent spokes were assessed through mass and energy balances, catalogued, and fed to the hub and spoke framework (Objective 4.3). These spokes resulted in a total of 14,580 unique value chain permutation;

an infeasible number to evaluate manually. In contrast, through application of the framework, objective LCIA results (spanning all three assessment strands and 19 indicators) for all 14,580 aggregated value chains were determined instantaneously, generating 277,020 data points (Objective 4.4). This represents what is by far the most comprehensive sustainability assessment of Hou process based soda ash value chains.

Objective 4.5, the last and perhaps most important, focusses on testing and evaluating the effectiveness of the framework's generation of recommendations through analysis of the proof-of-concept results. Initially, a broad view of the full permutation count was adopted. This showed that the reduction of impact indicator results to a single value through local normalisation, MCDM, and hub/spoke aggregation, delivered an approximately normally distributed set of overall subjective sustainability scores. This, along with the range (0.501), mean (0.588), and standard deviation (0.088) confirm effective utilisation of the available scoring bounds (0-1). In assessments with very high permutation counts, such as the proof-of-concept study herein, the generated scoring curve can be used to efficaciously screen out poorly performing options.

In addition to this screening capability, the frequency distribution of spoke selection within each set (relative to the permutation rankings) provides a quick and intuitive way of determining sensitive inputs. The resulting figures (6-32a-e) can be utilised in two ways; communication of results to non-practitioner decision makers, or by practitioners themselves as a jumping off point for deeper investigation or formal sensitivity analysis.

Returning to evaluation of the aggregated overall subjective sustainability scores, the relative influence of each indicator on permutation ranking was examined. Initially, this appeared to show that the framework generally prioritised the optimisation of LCA indicator performance over the other strands, despite the use of a neutral MCDM configuration (equal weightings for each indicator). However, when scrutinised further it was shown that this was in fact related to the standard deviation observed within each indicator across the 14,580 permutations. Subsequent quantitative evaluation showed that there is a strong correlation (0.8186) between the standard deviation of an indicators observed results and the alignment of local indicator ranking and global permutation rankings. This result demonstrates that the framework's underpinning methodology effectively accounts for the range of indicator magnitudes across the assessed spoke options; as discussed in Section 6.7.5.4, a hypothetical 2% reduction in GWP should not logically be prioritised over a potential 50% reduction in ODP when it comes to calculating competing value chains' overall subjective sustainability scores (assuming roughly equal indicator magnitudes and weightings).

Finally, the effects of MCDM configuration on the value chain recommendations are characterised. GWP was selected for this investigation due to its ubiquity within published sustainability assessments. Eight scenarios utilising GWP weightings between 0.052630 and 0.49091 were therefore examined. For each of these, the correlation between local indicator ranking and global permutation ranking was evaluated. This was repeated over the full range of permutations (14,580), as well as the top 10, 25, 50, 100, 500, 1000. This revealed that over the full range of permutations, the MCDM configuration had a weak effect on local vs global rankings. However, as the number of permutations included was reduced, the influence of the MCDM configuration increased, resulting in a perfect correlation for the top 10 recommendations in the three most heavily weighted scenarios. This behaviour is explained by the overall scoring profile (Figure 6-30). Where the highest and lowest performing permutations exhibit reasonably well differentiated overall subjective sustainability scores, these gaps decrease significantly as the mean score is approached. Consequently, a much larger GWP weighting would be required to align the local and global rankings and overcome the influence of the remaining 18 indicators.

In summary, the assessment architecture and characterisation models developed within this thesis have been proven to add value to the field. Deployment of the methodology within the FMCG space offers companies such as Unilever an opportunity to systematically evaluate potential value chains, both objectively and subjectively. The alignment of environmental, economic, and societal development with corporate strategy would undoubtably improve the pace with which we, as a society, can approach holistically sustainable industrial ecosystems. Furthermore, the developed approach to assessment improves the accessibility and communicability of strands, providing parallel results streams tailored for use by practitioners and decision makers respectively. Finally, the incorporated development of SIA characterisation models tackles a long persisting issue, previously preventing the meaningful integration of the strand with either LCA or TEA.

While all good LCAs, TEAs and SIAs deliver accurate yet imperfect representations of impact profiles, it is believed that this work effectively harnesses their respective strengths and capabilities to deliver holistic, useful, and actionable insights.

7.2 Future Work

Several developmental seams have been identified throughout this work, all of which would add tangible value to the presented methodology. These are summarised by the following list:

1. Incorporation of a tree network topology
2. Group based MCDM weighting derivation
3. Enhancement of OpEx calculations and associated insight generation
4. Sector specific SIA CMs based on the approach developed in Chapter 5

Firstly, the adoption of a tree network topology within a secondary methodology would allow for more comprehensive assessments of shorter value chains. This structure would facilitate the branching of supplier or route options at multiple points. However, this comes with limitations. As seen within the presented methodology, the number of permutations grows at a significantly faster rate than the number of spokes assessed. Adding additional hierarchical levels of spokes would exacerbate this issue. Despite this, for shorter value chains with only a handful of upstream steps, the granularity of insight generation would be greatly enhanced. Furthermore, the aggregation procedure of the current hub and spoke framework could be directly repurposed, accounting for the additional steps by scaling impact contributions via the product of the successive intermediate flows that lead to the primary hub. These single and multi-hub modelling approaches are analogous to the operability of system or unit LCIs within SimaPro LCAs. Single hub assessments deliver granularity in line with a system LCI based SimaPro model (aggregated LCIA profile for each spoke), whereas a multi-hub approach is analogous to a model built from unit LCIs (sub-divided LCIA for each hub input that details the impacts at each discrete value chain step).

The addition of group based MCDM would allow for the consideration multiple decision makers' opinions, achieving something approximating the Delphi technique. Due to the adoption of AHP-TOPSIS as the hub and spoke framework's MCDM methodology, this integration would be straight-forward. Group AHP has already been developed and utilised within literature, meaning that it could be cleanly swapped; also enabled by the presented methodologies partitioning of the weighting derivation (AHP) and ranking (TOPSIS) steps.

OpEx is clearly an important aspect of corporate decision making. Within this work it has been used as a proxy for the market price of feedstocks. This was required as market prices are not openly available for all technologies and routes. Furthermore, with current consumer pressure to make products sustainably, 'green' feedstocks often command premiums. In recognition of this weakness, an approach that adjusts the baseline OpEx to account for profits drawn at each preceding stage of the value chain would deliver a more representative 'at hub' cost. This could take the form of blanket compounding growth at each step, or a more sector specific and bespoke approach.

As identified within Chapters 5 and 6, the national level granularity of the developed SIA is a clear limitation; both in terms of insight generation and applicability. Enhancement of these models could feasibly allow for sector specificity. While it is not clear if the required data exists, the route to such models is far more transparent. For example, within the occupational safety and health indicator, the incident rate observed for different industrial sectors could be collated and normalised (placing the mean at a value of 1). These adjustment factors could then be applied to the national level indicator results in a similar fashion to that of Lang factors in TEA and process economics. The challenges are threefold; determining the most appropriate factor(s) through which to adjust the existing national level indicator scores, attaining data that achieves both accuracy and broad coverage, and determination of uncertainty.

In the end…

"All models are wrong, but some are useful"

George E. P. Box

[313]

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Appendix A

Table A-0-1 - Publications found through the systematic literature search and their associated characteristics.

#	Title	Year	MODM or MADM	MCDM Methodology	Reference	Inclusion?
1	Fuzzy CODAS Based Analysis of Wear and Temperature Induced Responses of Si Doped a-C film and CFRPEEK Tribopair	2022	MADM	Fuzzy-CODAS	[314]	No
2	Carbon Suitability Mapping for Forest Management Plan Decisions: The Case of Belgrade Forest (Istanbul)	2022	MADM	AHP	[315]	Yes
3	Embedding carbon impact assessment in multi-criteria supplier segmentation using ELECTRE TRI-rC	2022	MADM	ELECTRE	[316]	Yes
4	An application of the PROMETHEE II method for the comparison of energy requalification strategies to design Post-Carbon Cities	2022	MADM	PROMETHEE	[317]	No
5	Low-carbon tourism strategy evaluation and selection using interval-valued intuitionistic fuzzy additive ratio assessment approach based on similarity measures	2021	MADM	Fuzzy ARAS	[318]	No
6	Development and Utilization of Renewable Energy Based on Carbon Emission Reduction-Evaluation of Multiple MCDM Methods	2021	MADM	Review Paper	[319]	No
7	A Novel Methodology for Prioritizing Zero-Carbon Measures for Sustainable Transport	2021	MADM	BWM (Best Worst Model)	[320]	No
8	A multi-criteria analysis of forest restoration strategies to improve the ecosystem services supply: an application in Central Italy	2021	MADM	AHP	[321]	Yes
9	Novel q-rung orthopair fuzzy interaction aggregation operators and their application to low-carbon green supply chain management	2021	MADM	q-rung orthopair fuzzy number (q-ROFN)	[322]	No
10	Reconfiguring IVHF-TOPSIS decision making method with parameterized reference solutions and a novel distance for corporate carbon performance evaluation	2019	MADM	TOPSIS	[323]	Yes
11	Supportiveness of Low-Carbon Energy Technology Policy Using Fuzzy Multicriteria Decision-Making Methodologies	2020	MADM	AHP & TOPSIS (Fuzzy)	[324]	Yes
12	Technology selection for photovoltaic cell from sustainability perspective: An integrated approach	2020	MADM	Cloud Model and Grey Relational Analysis (CMGRA)	[325]	No
13	A low-carbon-orient product design schemes MCDM method hybridizing interval hesitant fuzzy set entropy theory and coupling network analysis	2019	MADM	Interval Hesitant Fuzzy Set Entropy (IHFSE)	[326]	No
14	Low-Carbon Energy Planning: A Hybrid MCDM Method Combining DANP and VIKOR Approach	2018	MADM	VIKOR and ANP	[327]	Yes
15	Decarbonization action plans using hybrid modelling for a low-carbon society: The case of Bangkok Metropolitan Area	2017	MODM?	Bilan Carbone Adaptation (not named)	[328]	No
16	Using Fuzzy DEA for Green Suppliers Selection Considering Carbon Footprints	2017	MADM	Revised DEA	[329]	No
17	A multi-criteria decision analysis on injection moulding of polymeric microcellular nanocomposite foams containing multi-walled carbon nanotubes	2017	MADM & MODM	AHP-TOPSIS & AHP-MOORA	[330]	No
18	Incorporating carbon footprint with activity-based costing constraints into sustainable public transport infrastructure project decisions	2016	MADM	DEMATEL, ANP, ZOGP	[331]	No
19	Hybrid Multi-criteria Decision-Making Approach for Supplier Evaluation in Fuzzy Environment	2016	MADM	TOPSIS-AHP	[332]	Yes

20	Scenarios for the future Brazilian power sector based on a multi criteria assessment	2016	Not specified	Multi-Criteria Decision Tool to Support Electricity Power Planning	[333]	No
21	A Multicriteria Decision Analysis Model and Risk Assessment Framework for Carbon Capture and Storage	2014	Not Specified	Risk Assessment developed from general MCDM principles	[334]	No
22	An Interdisciplinary Perspective on Carbon Capture and Storage Assessment Methods	2014	Review	Review Paper	[335]	No
23	Climate friendly technology transfer in the energy sector: A case study of Iran	2012	MADM	AHP	[336]	Yes
24	How Modelers Model: The Overlooked Social and Human Dimensions in Model Intercomparison Studies	2022	MADM	ANP, DEMATEL	[337]	No
25	Fixed-charge solid transportation problem with budget constraints based on carbon emission in neutrosophic environment	2022	MODM	Neutrosophic Linear Programming (NLP), Fuzzy Programming (FP) and Global Criterion Method (GCM)	[338]	No
26	Prioritizing transport planning strategies for freight companies towards zero carbon emission using ordinal priority approach	2022	MADM	Ordinal Priority Approach under picture fuzzy sets (OPA-P)	[339]	No
27	An integrated multi-granular distributed linguistic decision support framework for low carbon tourism attraction evaluation	2022	MADM	Organísation, rangement et Synthèse de données Relarionnelles (ORESTE)	[340]	No
28	A genetic algorithm tool for conceptual structural design with cost and embodied carbon optimization	2022	MODM	Non-dominated Sorted Genetic Algorithm II (NSGA-II)	[341]	No
29	A decision support system for sustainability prioritization of air pollution control technologies in energy and carbon management: Oil & gas industry of Iran	2022	MODM	ANP, DEMATEL, MULTIMOORA	[342]	No
30	An automotive radiator with multi-walled carbon-based nanofluids: A study on heat transfer optimization using MCDM techniques	2022	MADM	Entropy Technique, ARAS, CODAS	[343]	No
31	Carbon dioxide treatment method for autonomous underwater vehicles powered by direct methanol fuel cells: A multi-criteria decision analysis approach	2021	MADM	COPRAS, TOPSIS, AHP	[344]	Yes
32	Development and Utilization of Renewable Energy Based on Carbon Emission Reduction—Evaluation of Multiple MCDM Methods	2021	MADM	WSM, TOPSIS, PROMETHEE, ELECTRE, VIKOR	[345]	Yes
33	Technical, economic, carbon footprint assessment, and prioritizing stations for hydrogen production using wind energy: A case study	2021	MADM	SWARA-EDAS hybrid	[346]	Yes
34	Evaluating carbon capturing strategies for emissions reduction in community energy systems: A life cycle thinking approach	2021	MADM	VIKOR	[347]	Yes
35	Reducing carbon dioxide emissions from electricity sector using demand side management	2021	MADM	AHP	[348]	Yes
36	Low-carbon tourism destination selection by a thermodynamic feature-based method	2021	MADM	q-rung orthopair fuzzy set (Q-ROFS)	[349]	No
37	The Analysis of Small Investors' Demands on a Thermal Insulation System for a Family House: A Case Study	2021	MADM	method of the basic variant	[350]	N0
38	Sustainable Evaluation of Using Nano Zero-Valent Iron and Activated Carbon for Real Textile Effluent Remediation	2020	MADM	AHP, TOPSIS, SAW	[351]	Yes
39	Reconfiguring IVHF-TOPSIS decision making method with parameterized reference solutions and a novel distance for corporate carbon performance evaluation	*Duplicate*				
40	Intuitionistic Fuzzy Hierarchical Multi-Criteria Decision Making for Evaluating Performances of Low-Carbon Tourism Scenic Spots	2020	MADM	Intuitionistic fuzzy hierarchical MCDM	[352]	No

41	Use and misuse of the net present value in environmental studies	2020	N/A	Not specified	[353]	No
42	Technology selection for photovoltaic cell from sustainability perspective: An integrated approach	*Duplicate*				
43	Low carbon supplier development: A fuzzy c-means and fuzzy formal concept analysis based analytical model	2019	MADM	fuzzy c-means and fuzzy formal concept analysis based analytical model	[354]	No
44	An application of the Analytic Hierarchy Process for prioritizing user preferences in the design of a Home Energy Management System	2018	MADM	AHP	[355]	Yes
45	Development of an MCDM framework to facilitate low carbon shipping technology application	2018	MADM	multi-aspect framework to support the LCS decision-making process	[356]	No
46	Material selection for automated dry fibre placement using the analytical hierarchy process	2018	MADM	AHP	[357]	No
47	Prioritizing mechanism of low carbon shipping measures using a combination of FQFD and FTOPSIS	2017	MADM	Quality Function Deployment (QFD), TOPSIS	[358]	Yes
48	An integrated buyer initiated decision-making process for green supplier selection	2016	MADM	CMS-GDEA	[359]	No
49	Systematic Framework for Design of Environmentally Sustainable Pharmaceutical Supply Chain Network	2016	MADM	AHP	[360]	Yes
50	Duplicate (Hybrid Multi-criteria Decision-Making Approach for Supplier Evaluation in Fuzzy Environment)	*Duplicate*				
51	Assessing Complexity of Carbon Capture and Storage using Multi-Criteria Decision-Making Methods	2015	MADM	AHP, DEMATEL	[361]	Yes
52	Carbon Suitability Mapping for Forest Management Plan Decisions: The Case of Belgrade Forest (Istanbul)	*Duplicate*				
53	Multi-criteria screening of carbon dioxide utilization products combined with process optimization and evaluation	2022	MADM	TOPSIS	[362]	Yes
54	Allocation of provincial carbon emission allowances under China's 2030 carbon peak target: A dynamic multi-criteria decision analysis method	2022	MADM	DEA	[363]	Yes
55	A genetic algorithm tool for conceptual structural design with cost and embodied carbon optimization	*Duplicate*				
56	An application of the PROMETHEE II method for the comparison of energy requalification strategies to design Post-Carbon Cities	*Duplicate*				
57	Multidimensional assessment of the energy sustainability and carbon pricing impacts along the Belt and Road Initiative	2022	MADM	PROMETHEE	[364]	Yes
58	Multi-criteria Decision-making in Carbon-Constrained Scenario for Sustainable Production Planning	2021	MADM	TOPSIS	[365]	Yes
59	Multi-criteria decision approach to select carbon dioxide and hydrogen sources as potential raw materials for the production of chemicals	2021	MADM	TOPSIS	[366]	Yes
60	Multi criteria decision analysis for screening carbon dioxide conversion products	2021	MADM	TOPSIS	[367]	Yes
61	Long-term impacts of increased timber harvests on ecosystem services and biodiversity: A scenario study based on national forest inventory data	2020	MADM	SMART	[368]	No
62	Technology selection for photovoltaic cell from sustainability perspective: An integrated approach	*Duplicate*				
63	Advances and challenges of implementing carbon offset mechanism for a low carbon economy: The Taiwanese experience	2019	MADM	AHP, TOPSIS	[369]	Yes

64	Supporting Europe's Energy Policy Towards a Decarbonised Energy System: A Comparative Assessment	2019	MADM	PROMETHEE	[370]	Yes
65	Low carbon supplier development: A fuzzy c-means and fuzzy formal concept analysis based analytical model	*Duplicate*				
66	Assessment of the impact of progressive carbon taxation strategies on Supply Chain's strategic decisions and performances	2019	MODM	mixed-integer non-linear program (MINLP)	[371]	No
67	Segregated versus integrated biodiversity conservation: Value-based ecosystem service assessment under varying forest management strategies in a Swiss case study	2018	MODM	Multi Attribute Value Theory (MAVT)	[372]	No
68	A multi-criteria decision analysis model for carbon emission quota allocation in China's east coastal areas: Efficiency and equity	2017	MADM	WSM	[373]	Yes
69	Duplicate (Scenarios for the future Brazilian power sector based on a multi criteria assessment)	*Duplicate*				
70	Interdisciplinary assessment of renewable, nuclear, and fossil power generation with and without carbon capture and storage in view of the new Swiss energy policy	2016	MADM	WSM	[150]	Yes
71	An integrated buyer initiated decision-making process for green supplier selection	*Duplicate*				
72	Hybrid Multi-criteria Decision-Making Approach for Supplier Evaluation in Fuzzy Environment	*Duplicate*				

Table A-0-2 - MADM methodological distribution across the publications included from the systematic literature search

Method	***Frequency***	***References***
AHP	11	[315], [321], [324], [332], [336], [344], [348], [351], [355], [360], [369]
ELECTRE	2	[316], [345]
TOPSIS	13	[323], [324], [332], [344], [345], [351], [358], [361], [362], [365], [366], [367], [369]
VIKOR	3	[327], [345], [347]
WSM	3	[345], [373], [150]
PROMETHEE	3	[345], [364], [370]
ANP	1	[327]
DEMATEL	1	[361]
COPRAS	1	[344]
SWARA-EDAS hybrid	1	[346]
SAW	1	[351]
QFD	1	[358]
Data Envelope Analysis (DEA)	1	[363]

Table A-0-3 - publications included, excluded (with reasoning) from the systematic literature search

Result	***Reason***	***Count***	***Reference***
Excluded	Review	2	[319], [335]
	Scope (CCU/CCS)	14	[314], [317], [325], [330], [337], [338], [343], [350], [352], [353], [357], [368], [371], [372]
	Novel Methodology Proposal	15	[318], [320], [322], [326], [328], [329], [331], [339], [340], [341], [342], [349], [354], [356], [359]
	Duplicate	11	[325], [332], [315], [341], [317], [325], [354], [333], [359], [332], [323]
	Methodology not named	2	[334], [333]
Included	Criteria Met	28	[315], [316], [321], [323], [324], [327], [332], [336], [344], [345], [346], [347], [348], [351], [355], [358], [360], [361], [362], [363], [364], [365], [366], [367], [369], [370], [373], [150]

Table A-0-4 - Methodological advantages and disadvantages for MADM techniques employed in CDU relevant publications

MADM Technique	Advantages	Disadvantages
TOPSIS [162]	1. Weightings are the only subjective inputs [165] 2. Less "human" input than many other methodologies [178], reducing scope for bias 3. Capable of handling very large numbers of alternatives with high computational efficiency [165] 4. Procedural complexity does not change as number of criteria increases 5. Does not require that all criteria have a scoring scale with the same directionality. That is, a high score does not have to always mean better performance. 6. Intuitive and clear logic [165] 7. Possibility for visualisation [165]	1. Does not incorporate criteria weighting calculation in standard methodology 2. No user input consistency checks [165] 3. Susceptible to rank reversal phenomena [166] 4. Finds ideal solution based on the closest distance to the positive ideal solution and farthest distance from the negative ideal solution. However, the relative importance of these distances is not considered through weighting [164] [160] 5. Requires all data points are known and crisp [165]
Analytical Hierarchy Process [196]	1. Most commonly used method within MCDM [374] 2. Developed for complex decision-making problems [178] 3. Allows for finer control and monitoring of decision-making consistency (both for individual assessors and groups) [168] [169] 4. Facilitates groups of assessors/decision makers [170] [171] 5. Handles a reasonable number of criteria that cannot be ranked directly with ease [375] 6. Tiered approach can be used to aid with clarity of decision maker value choices and issues around input consistency 7. Suited to the allocation of resources and business effort [172] 8. Appropriate for the integration of qualitative data [163] [173] 9. Handles subjective assessment well within academic applications [376] 10. Provides transparent criteria weightings [196] [207]	1. Constrained to a reasonable number of criteria [178], ensuring that consistency requirements can still be met 2. Requires a (potentially large) number of pairwise comparisons [178] 3. Focussed primarily on hierarchical decision problems [163] 4. Applied weightings can have significant influence on final score or recommendation [174] (these points and potential resolutions are explored in literature [175] [176]).
Weighted Sum Model [377]	1. Simple methodology 2. Results can be obtained very quickly 3. Highly transparent approach and calculations 4. Broad applicability to many problems	1. Human perception and logic of prioritisation is prone to errors when more than four criteria are present [191] 2. Direct weighting application by practitioners invites bias (conscious or unconscious) 3. Fails to define interrelations between criteria [178] 4. Requires that all criteria inputs share a common unit, or inputs are normalised relative to prescribed bounds. 5. A small change in in weights may results in big changes in the objective vectors [179] 6. Calculated optimal solution can be inappropriate due to excluded study aspects or weighting errors [378] 7. Radically different criteria weightings can produce the same objective vector [179] 8. Not appropriate for mixed optimisation problems (criteria must all be seeking maximum or all seeking minimum values)
VIKOR [379]	1. Accepts conflicting criteria [380] 2. Handles large numbers of alternatives 3. Methodology is conceptually intuitive [180]	1. Often results in erroneous alternative rankings due to method of calculation for the maximum group utility and the minimum individual regret of the opponent [181] 2. No effective weighting determination, requiring combination with other techniques for accurate and stable results [182]
PROMETHEE	1. Few user inputs required compared to other methodologies [184] 2. No requirement for criteria / indicator score normalisation [163] 3. Includes four sub-methodologies tailored to specific applications (PROMETHEE I, PROMETHEE II, PROMETHEE III, AND PROMETHEE IV) [381] [382] 4. Stable with respect to minor changes to inputs	1. No weighting technique is included in the method [383] 2. Does not aid with problem structure identification [184] 3. Often exhibits loss of data or resolution if used to generate complete rankings [184] 4. Suffers from rank reversal phenomena [185]

	5. Criteria scale directionality can vary. This is accounted for through differentiated normalisation procedure for beneficial and non-beneficial criteria.	
ELECTRE	1. Accounts for uncertainty and imprecision 2. Allows for the prescription of ‘veto’ criteria, removing undesirable alternatives [188] 3. Applicable to decision making scenarios with multiple stakeholders [188] 4. Handles problems with many comparison criteria [384] 5. Seven sub-methodologies are present (ELECTRE I, ELECTRE Iv, ELEC- TRE IS, ELECTRE II, ELECTRE III, ELECTRE IV, ELECTRE TRI) [186], tailoring the approach to different problem types 6. Does not require that all alternatives and criteria are characterised on the same scale [384]	1. Requirement of an additional discrimination (veto) threshold; ranking of the alternative depends on the size of this threshold for which there exists no ‘correct’ value [163]. 2. Significant workload requirements [189] 3. Methodology is difficult to explain and unintuitive

Work Cited (Appendix A):

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Appendix B

Spoke Data Sheet
(Insert Spoke Name)

Inventory Overview:

Quantity:	Character:
Input or Output?	-
Local Functional Unit	-
Scope	-
Geographic Region	-
Timeframe	-

System Boundary Block Flow Diagram (BFD):

(Insert system boundary diagram)

Spoke Description:

(Insert technology and system description)

Boundary Flows:

Classification:	Type:	Description:	Notation:
Input(s)	-	-	-
	-	-	-
Output(s)	-	-	-
	-	-	-

Process Units Included:

Classification:	Type:	Description:
Primary	-	-
	-	-
	-	-
Secondary	-	-
	-	-
	-	-
	-	-
	-	-

Assumptions:

Aspect:	Assumption(s):
System Boundary	• -
Mass balance	• -
Energy balance	• -
Waste handling	• -
Transportation	• -
Miscellaneous	• -

Stream Table:

Stream	Species (kmol/hr)								Species (kg/hr)								Total
	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Lifecycle Assessment (LCA) Data:

Indicator	Value	Unit
Global Warming Potential (GWP)	-	kg CO_2-eq. / FU
Ozone Depletion	-	kg CFC-11-eq. / FU
Metal Resource Depletion	-	kg Cu-eq. / FU
Freshwater Eutrophication Potential	-	kg P-eq. / FU
Marine Eutrophication Potential	-	kg N-eq. / FU
Acidification Potential	-	kg SO_2-eq. / FU
Water Use	-	m^3 / FU

Technoeconomic Assessment (TEA) Data

Variable	Value	Unit
-	-	MJ / FU
-	-	MJ / FU
-	-	MJ / FU
Total:	-	MJ / FU

Variable	Value	Unit
-	-	-
-	-	-
-	-	-
Overall Relative Energy Efficiency:	-	Decimal

Variable	Value	Unit
-	-	kg / FU
-	-	kg / FU
-	-	Decimal
-	-	Decimal
Overall Relative Mass Efficiency:	-	Decimal

Flow	Price Data / FU	Data Currency	Year	Price 2022£ / FU:	Quantity Req. (FU):	Total Value:	Unit
-	-	-	-	-	-	-	£ / FU
					Total:	-	£ / FU

Social Impact Assessment (SIA) Data:

Indicator	Sub-Indicator(s)	Sub-Indicator Value(s)	Final Aggregated Indicator Score
Occupational Health and Safety (OSH)	Accidents causing >4 days' absence	-	-
	Work-related disease	-	
	Work-related mortality	-	
Child Labour	Non-hazardous	-	-
	Hazardous		
	Vulnerability	-	
Forced Labour	Prevalence	-	-
	Vulnerability	-	
Access to Electricity	Energy imports, net (% of energy use)	-	-
	Fossil fuel energy consumption (% of total)	-	
	Electric power consumption (kWh per capita)	-	
	Renewable energy consumption (% of total final energy consumption)	-	
Access to Water	Freshwater withdrawal as % of total	-	-
	Water Stress	-	
Land Use Change	-	-	-
Utilisation of Hazardous Materials	Deaths caused by dangerous substances per 10,000 workers	-	-

Aggregated Final Objective Indicator Scores:

Assessment Strand:	Indicator:	Value:	Units:
LCA	Global Warming Potential (GWP)	-	kg CO_2-eq. / FU
	Ozone Depletion	-	kg CFC-11-eq. / FU
	Metal Resource Depletion	-	kg Cu-eq. / FU
	Freshwater Eutrophication Potential	-	kg P-eq. / FU
	Marine Eutrophication Potential	-	kg N-eq. / FU
	Acidification Potential	-	kg SO_2-eq. / FU
	Water Use	-	m^3 / FU
TEA	Energy Demand	-	MJ / FU
	Energy Efficiency (%)	-	%
	Mass Efficiency (%)	-	%
	Est. Purchase Price (2022 £)	-	2022 £ / FU
SIA	Occupational Health and Safety (OSH)	-	-
	Child Labour	-	-
	Forced Labour	-	-
	Access to Electricity	-	-
	Access to Water	-	-
	Land Use Change	-	-
	Utilisation of Hazardous Materials	-	-

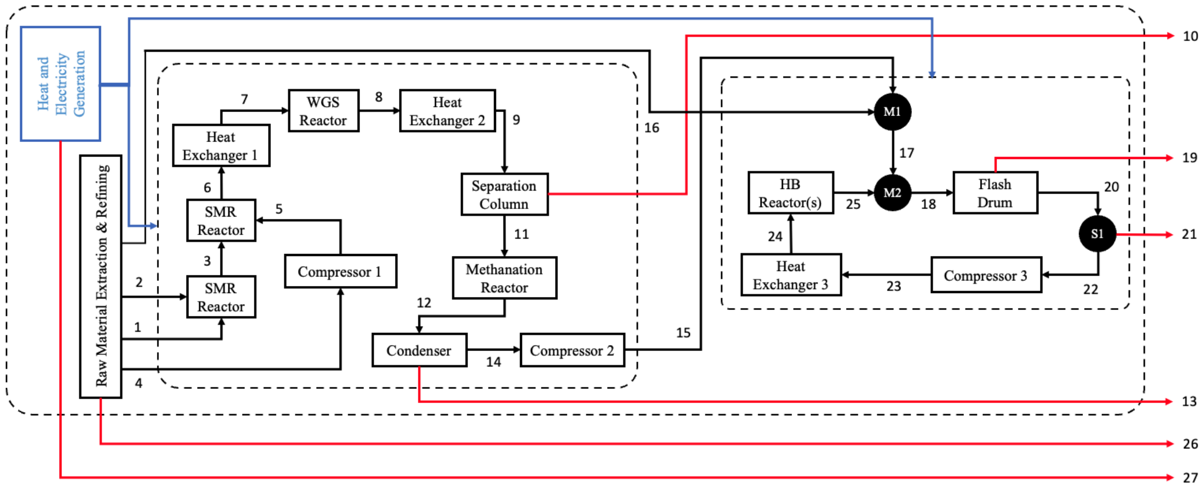
Appendix C

Spoke Data Sheet (I.D. 1.1)
(NH_3 from Steam Methane Reformation & Haber Bosch)

Inventory Overview:

Quantity:	Character:
Input or Output?	Input
Reference Flow	1 tonne NH_3 via Steam Methane Reformation & Haber Bosch
Scope	Cradle-to-Gate
Geographic Region	India
Timeframe	2022

System Boundary Block Flow Diagram (BFD):



Spoke Description:

This cradle-to-grave assessment of ammonia production assesses the coupled use of steam methane reforming and the Haber-Bosch process. It is assumed that all process heat (values obtained from literature) is provided through the combustion of methane. Steam methane reformation and Haber-Bosch models from the literature are identified for use (see table below). The impacts of raw material extraction and preparation for the process are examined using the appropriate Ecoinvent data sets and added to the direct emission associated with process operation.

Spoke Sub-Section	Literature / Models Employed
Steam Methane Reformation	[376] [377] [378] [379]
Haber-Bosch Process	[380] [381] [382]

In the first modelled step, hydrogen is produced from methane and, in the second, ammonia is synthesised via the Haber–Bosch reaction. Hydrogen is produced by primary and secondary steam methane reforming reactors (SMR) (Equation C-1). The first SMR reactor operates at around 850–900°C and 25–35 bar with the energy required for the endothermic reaction being provided by the combustion of methane. The second SMR reactor is autothermal, air is compressed and fed to the reactor to provide heat of reaction by partial oxidation of the reagents at 900–1000°C.

Equation C-1

$$CH_4 + H_2O \leftrightarrow CO + 3H_2O$$

The SMR outlet mixture of carbon monoxide, hydrogen, and unreacted steam and methane are introduced into the two-stage water–gas shift (WGS) reactor to maximise CO conversion to hydrogen. The WGS reaction is exothermic, and heat must be removed to minimise CO concentration at equilibrium.

Equation C-2

$$CO + H_2O \leftrightarrow CO_2 + H_2$$

The residual CO and CO2 in the H2-nitrogen mixture must be removed since they poison the HB catalyst.4 Hence, a methanation unit was placed after the MEA absorber to convert the residual CO and CO_2 to methane and water. The vapour outlet of the absorption column is heated to 230 °C and fed to the methanation unit, which is modelled as a plug flow reactor implementing Equation C-3 & Equation C-4. The residual methane present accumulates in the downstream synthesis loop (argon is also present but not modelled due to its presence in negligible mole fractions and removal in a purge stream).

Equation C-3

$$CO + 3H_2 \leftrightarrow CH_4 + H_2O$$

Equation C-4

$$CO_2 + 4H_2 \leftrightarrow CH_4 + 2H_2O$$

Although the steam methane reforming reactions are endothermic, the high reaction temperature and the need to cool substantially for the water gas shift reaction means that there is substantial waste heat available. This heat is used for raising high-pressure steam, which is expanded in steam turbines for compression, mainly used for compression of the feed in the Haber Bosch loop and the reformer combustion air compressor, which are the largest two energy users. The use of methane as feedstock inevitably leads to significant CO2 emissions from the process, and this is further compounded by the use of methane as fuel for the primary reformer furnace. The reaction kinetics are reported in Herwijnen et al. (1973), At the selected operating pressure, the conversion of CO2 and CO is 100%.

The H2 mixture is compressed to 196.3 bar, mixed with the recycle stream from the NH3 reactor, and then sent to a flash operating at the same pressure and 42 °C. The liquid outlet, rich in NH3, is sent to a flash unit, reaching an NH3 purity of ~98 mol% at the bottom.

The Haber-Bosch reaction system is modelled as a series of adiabatic plug-flow reactors with a void fraction of 33%, loaded with an iron-based catalyst. The kinetic model of the main reaction was directly adapted from the original reference (Morud & Skogestad, 1998) (Equation 0-5).

Equation 0-5

$$N_2 + 3H_2 \leftrightarrow 2NH_3$$

A nitrogen conversion of 25.3% is achieved inside the reactor. The reactor outlet is then cooled down to 27.1 °C and mixed with the fresh feed. It is then sent to the first flash, separating NH_3 from the remaining compounds and closing the loop.

Boundary Flows:

Classification:	Type:	Description:	Notation:
Input(s)	Raw material extraction	Ecoinvent used to evaluate the impact of feedstock extraction from the environment	N/A
Output(s)	Stream 10	CO_2 purge from WGS	10
	Stream 13	Water outlet from condenser	13
	Stream 19	Ammonia product (liquid)	19
	Stream 21	Haber Bosch loop purge stream	21
	Stream 26	Impacts and emissions associated with raw material extraction and preparation	26
	Stream 27	Impacts associated with the construction and operation of methane fired heating equipment	27

Process Units Included:

Classification:	Type:	Description:
Primary	SMR 1	First SMR, operating at 60% conversion
	SMR 2	Second SMR, achieving a 96.1% overall efficiency
	WGS Reactor	Conversion of CO to CO_2 through the
	Separation Column	Removes CO_2 from the WGS product stream
	Methanation Reactor	Converts remaining traces of CO and CO_2 back to CH_4 to prevent catalyst poisoning within the downstream HB reactor
	HB Reactor	Production of ammonia with a recycle loop to improve efficiency.
Secondary	HX 1	-
	Compressor 1	-
	HX2	-
	Condenser	-
	Compressor 2	-
	Mixer 1	-
	Mixer 2	-
	Flash Drum	-
	Splitter 1	-
	Compressor 3	-
	HX 3	-

Assumptions:

Aspect:	Assumption(s):

System Boundary	• Ecoinvent datasets assumed to be reflective of the secondary feedstock production (ReCiPe Midpoint (H) characterisation)
	• Electricity generation is handled on-site via a steam turbine fed by process steam from methane combustion
	• Heat is supplied via methane combustion
	  ○ Mol/m3 supplied is evaluated using ideal gas law (5 Bar, 298.15 K)
	  ○ 4.5 GJ / tonne NH_3 heat requirement (German UBA, 2000) [384]
	• CO_2 removal within SMR is achieved using Selexol due to its widespread adoption (European Union Joint Research Council, 2007)
	• US natural gas production data used to estimate BAT, as global averages are not available.
	• Excludes SMR/HB plant construction & decommissioning
	• Costing data taken from literature for grey ammonia (natural gas fed without CCS) in Asia (S&P Global Commodity Insights, 2023)

Mass balance	• 60% conversion efficiency within primary SMR (European Union Joint Research Council, 2007) • 96.1% conversion efficiency within second SMR (derived from mass balance and primary data for outlet stream composition) (European Union Joint Research Council, 2007) • Steam to methane ratio of 3:1 (European Union Joint Research Council, 2007) • 98% conversion within WGS reactor (European Union Joint Research Council, 2007) • 100% CO & CO_2 conversion efficiency within methanation reactor (D'Angelo, et al., 2021) • Emissions calculations from methane combustion for steam generation assume an optimal 90% combustion efficiency (Mickey, 2017) and 84.3% heat recovery (Najmi & Arhosazni, 2006)
Energy balance	• Average values for BAT plants (29.6 GJ/tonne NH_3) taken from an LCA/TEA with matching system boundaries [384]. This was then sense checked against a consideration of minimum energy required through enthalpy calculations. Energy supplied by menthane in SMR reactions is subsequently excluded as impacts are captured by the process' mass balance.

	• Methane energy content of 52 MJ/kg and sourcing from natural gas (fossil) • Energy efficiency of methane burners assumed to be 90% as detailed in literature (Mickey, 2017)
Waste handling	• Gaseous emissions are directly vented. • Liquid effluents released to waterways.
Transportation	• Not included
Miscellaneous	• None

Stream Table:

Stream	Species In (kmol/hr)							Species In (kg/hr)							Totals
	CH4	H2O	CO	H2	CO2	N2	NH3	CH4	H2O	CO	H2	CO2	N2	NH3	
1	23.09642168	0	0	0	0	0	0	369.542747	0	0	0	0	0	0	369.542747
2	0	69.289265	0	0	0	0	0	0	1247.206771	0	0	0	0	0	1247.206771
3	9.238568672	55.431412	13.85785301	41.573559	0	0	0	147.817099	997.7654166	388.019884	83.147118	0	0	0	1616.749518
4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.000000
5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.000000
6	0.360304178	46.5531475	22.7361175	68.2083525	0	0	0	5.76486685	837.9566557	636.61129	136.416705	0	0	0	1616.749518
7	0.360304178	46.5531475	22.7361175	68.2083525	0	0	0	5.76486685	837.9566557	636.61129	136.416705	0	0	0	1616.749518
8	0.360304178	24.2717524	0.45472235	90.4897477	22.28139515	0	0	5.76486685	436.891543	12.7322258	180.979495	980.381387	0	0	1616.749518
9	0.360304178	24.2717524	0.45472235	90.4897477	22.28139515	0	0	5.76486685	436.891543	12.7322258	180.979495	980.381387	0	0	1616.749518
10	0	0	0	0	22.28139515	0	0	0	0	0	0	980.381387	0	0	980.381387
11	0.360304178	24.2717524	0.45472235	90.4897477	0	0	0	5.76486685	436.891543	12.7322258	180.979495	0	0	0	636.368131
12	0.815026528	24.7264747	0	89.1255806	0	0	0	13.0404245	445.0765453	0	178.251161	0	0	0	636.368131
13	0	24.7264747	0	0	0	0	0	0	445.0765453	0	0	0	0	0	445.076545
14	0.815026528	0	0	89.1255806	0	0	0	13.0404245	0	0	178.251161	0	0	0	191.291586
15	0.815026528	0	0	89.1255806	0	0	0	13.0404245	0	0	178.251161	0	0	0	191.291586
16	0	0	0	0	0	29.7364711	0	0	0	0	0	0	832.621191	0	832.621191
17	0.815026528	0	0	89.1255806	0	29.7364711	0	13.0404245	0	0	178.251161	0	832.621191	0	1023.912777
18	20.34251538	0	0	369.536571	0	108.493132	139.26747	325.480246	0	0	739.073141	0	3037.8077	2367.546998	6469.908089
19	0	0	0	0.8412385	0	0.3094244	58.8235294	0	0	0	1.682477	0	8.6638833	1000	1010.346360
20	20.34251538	0	0	368.695332	0	108.183708	80.4439411	325.480246	0	0	737.390664	0	3029.14382	1367.546998	5459.561729
21	0.815026528	0	0	0.03784118	0	0.0114979	0.00771378	13.0404245	0	0	0.07568236	0	0.3219411	0.131134237	13.569182
22	19.52748885	0	0	368.657491	0	108.17221	80.4362273	312.439822	0	0	737.314982	0	3028.82188	1367.415864	5445.992546
23	19.52748885	0	0	368.657491	0	108.17221	80.4362273	312.439822	0	0	737.314982	0	3028.82188	1367.415864	5445.992546
24	19.52748885	0	0	368.657491	0	108.17221	80.4362273	312.439822	0	0	737.314982	0	3028.82188	1367.415864	5445.992546
25	19.52748885	0	0	280.41099	0	78.7566611	139.26747	312.439822	0	0	560.82198	0	2205.18651	2367.546998	5445.995312
26	Boundary flow with impacts assessed through Ecoinvent data set: 'natural gas production - US - natural gas, high pressure'														N/A
27	Boundary flow with impacts assessed through Ecoinvent data set: 'natural gas production - US - natural gas, high pressure' & stochiometric evaluation of emissions (CH4 & CO2)														N/A

Lifecycle Assessment (LCA) Data:

Indicator	Value	Unit
Global Warming Potential (GWP)	1998.817114	kg CO_2-eq. / FU
Ozone Depletion	0.000001	kg CFC-11-eq. / FU
Mineral Resource Depletion	1.374034	kg Cu-eq. / FU
Freshwater Eutrophication Potential	0.003315	kg P-eq. / FU
Marine Eutrophication Potential	0.013564	kg N-eq. / FU
Acidification Potential	0.040155	kg SO_2-eq. / FU
Water Use	1.297039	m^3 / FU

Technoeconomic Assessment (TEA) Data:

Variable	Value	Unit
Energy Requirement	26,900	MJ / FU
Total:	26,900	MJ / FU

Variable	Value	Unit
Energy Input	5,000	MJ / FU
Theoretical Energy Requirement	4,500	MJ / FU
Achieved Energy Efficiency	0.9	Decimal
Overall Relative Mass Efficiency:	0.9	Decimal

Variable	Value	Unit
Mass Fed (Total)	2449.37	kg / FU
Mass of Product	1000	kg / FU
Theoretical Maximum Mass Efficiency	0.4157	Decimal
Achieved Mass Efficiency	0.4083	Decimal
Overall Relative Mass Efficiency:	0.982	Decimal

Flow	Price Data	Data Currency	Year	Price 2022£ / FU:	Quantity Req.:	Total Value:	Unit
1 Tonne	655	USD	2023 (Oct)	517.45	1	517.45	£ / FU
					Total:	517.45	£ / FU

Social Impact Assessment (SIA) Data:

Indicator	Sub-Indicator(s)	Sub-Indicator Value(s)	Final Aggregated Indicator Score
Occupational Health and Safety (OSH)	Accidents causing >4 days' absence	0.586213385	0.611831817
	Work-related disease	0.754901847	
	Work-related mortality	0.714012633	
Child Labour	Non-hazardous	0.740585774	0.607493035
	Hazardous		
	Vulnerability	0.493530724	
Forced Labour	Prevalence	0.973555901	0.69338248591082
	Vulnerability	0.493530724	
Access to Electricity	Energy imports, net (% of energy use)	0.849781993	0.476854933524488
	Fossil fuel energy consumption (% of total)	0.123295692	
	Electric power consumption (kWh per capita)	0.070600891	
	Renewable energy consumption (% of total final energy consumption)	0.1445	
Access to Water	Freshwater withdrawal as % of total	0.791635859	0.498116751
	Water Stress	0.567783117	
Land Use Change	-	0.277838446	0.194659486476648
Utilisation of Hazardous Materials	Deaths caused by dangerous substances per 10,000 workers	0.754900315	0.591436178275647

Aggregated Final Objective Indicator Scores:

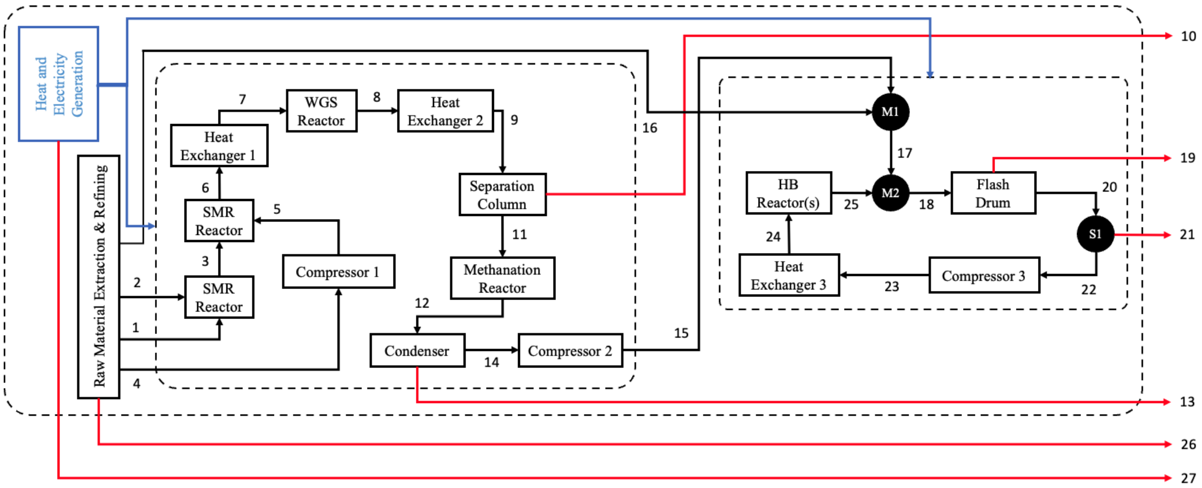
Assessment Strand:	Indicator:	Value:	Units:
LCA	Global Warming Potential (GWP)	1998.817114	kg CO_2-eq. / FU
	Ozone Depletion	0.000001	kg CFC-11-eq. / FU
	Mineral Resource Depletion	1.374034	kg Cu-eq. / FU
	Freshwater Eutrophication Potential	0.003315	kg P-eq. / FU
	Marine Eutrophication Potential	0.013564	kg N-eq. / FU
	Acidification Potential	0.040155	kg SO_2-eq. / FU
	Water Use	1.297039	m^3 / FU
TEA	Energy Demand	26,900	MJ / FU
	Energy Efficiency (%)	0.9	%
	Mass Efficiency (%)	0.982	%
	Est. Purchase Price (2022 £)	517.45	2022 £ / FU
SIA	Occupational Health and Safety (OSH)	0.611831817	-
	Child Labour	0.607493035	-
	Forced Labour	0.693382486	-
	Access to Electricity	0.476854934	-
	Access to Water	0.498116751	-
	Land Use Change	0.194659486	-
	Utilisation of Hazardous Materials	0.591436178	-

Spoke Data Sheet (I.D. 1.2)
(NH_3 from Steam Methane Reformation & Haber Bosch)

Inventory Overview:

Quantity:	Character:
Input or Output?	Input
Reference Flow	1 tonne NH_3 via Steam Methane Reformation & Haber Bosch
Scope	Cradle-to-Gate
Geographic Region	India
Timeframe	2022

System Boundary Block Flow Diagram (BFD):



Spoke Description:

This cradle-to-grave assessment of ammonia production assesses the coupled use of steam methane reforming and the Haber-Bosch process. It is assumed that all process heat (values obtained from literature) is provided through the combustion of methane. Steam methane reformation and Haber-Bosch models from the literature are identified for use (see table below). The impacts of raw material extraction and preparation for the process are examined using the appropriate Ecoinvent data sets and added to the direct emission associated with process operation.

Spoke Sub-Section	Literature / Models Employed
Steam Methane Reformation	[376] [377] [378] [379]
Haber-Bosch Process	[380] [381] [382]

In the first modelled step, hydrogen is produced from methane and, in the second, ammonia is synthesised via the Haber–Bosch reaction. Hydrogen is produced by primary and secondary steam methane reforming reactors (SMR) (Equation C-1). The first SMR reactor operates at around 850–900°C and 25–35 bar with the energy required for the endothermic reaction being provided by the combustion of methane. The second SMR reactor is autothermal, air is compressed and fed to the reactor to provide heat of reaction by partial oxidation of the reagents at 900–1000°C.

Equation 0-6

$$CH_4 + H_2O \leftrightarrow CO + 3H_2O$$

The SMR outlet mixture of carbon monoxide, hydrogen, and unreacted steam and methane are introduced into the two-stage water–gas shift (WGS) reactor to maximise CO conversion to hydrogen. The WGS reaction is exothermic, and heat must be removed to minimise CO concentration at equilibrium.

Equation 0-7

$$CO + H_2O \leftrightarrow CO_2 + H_2$$

The residual CO and CO2 in the H2-nitrogen mixture must be removed since they poison the HB catalyst. Hence, a methanation unit was placed after the MEA absorber to convert the residual CO and CO2 to methane and water. The vapour outlet of the absorption column is heated to 230 °C and fed to the methanation unit, which is modelled as a plug flow reactor implementing Equation C-3 & Equation C-4. The residual methane present accumulates in the downstream synthesis loop (argon is also present but not modelled due to its presence in negligible mole fractions and removal in a purge stream).

Equation 0-8

$$CO + 3H_2 \leftrightarrow CH_4 + H_2O$$

Equation 0-9

$$CO_2 + 4H_2 \leftrightarrow CH_4 + 2H_2O$$

Although the steam methane reforming reactions are endothermic, the high reaction temperature and the need to cool substantially for the water gas shift reaction means that there is substantial waste heat available. This heat is used for raising high-pressure steam, which is expanded in steam turbines for compression, mainly used for compression of the feed in the Haber Bosch loop and the reformer combustion air compressor, which are the largest two energy users. The use of methane as feedstock inevitably leads to significant CO2 emissions from the process, and this is further compounded by the use of methane as fuel for the primary reformer furnace. The reaction kinetics are reported in Herwijnen et al. (1973), At the selected operating pressure, the conversion of CO2 and CO is 100%.

The H2 mixture is compressed to 196.3 bar, mixed with the recycle stream from the NH3 reactor, and then sent to a flash operating at the same pressure and 42 °C. The liquid outlet, rich in NH3, is sent to a flash unit, reaching an NH3 purity of ~98 mol% at the bottom.

The Haber-Bosch reaction system is modelled as a series of adiabatic plug-flow reactors with a void fraction of 33%, loaded with an iron-based catalyst. The kinetic model of the main reaction was directly adapted from the original reference (Morud & Skogestad, 1998) (Equation 0-5).

Equation 0-10

$$N_2 + 3H_2 \leftrightarrow 2NH_3$$

A nitrogen conversion of 25.3% is achieved inside the reactor. The reactor outlet is then cooled down to 27.1 °C and mixed with the fresh feed. It is then sent to the first flash, separating NH_3 from the remaining compounds and closing the loop.

Boundary Flows:

Classification:	Type:	Description:	Notation:
Input(s)	Raw material extraction	Ecoinvent used to evaluate the impact of feedstock extraction from the environment	N/A
Output(s)	Stream 10	CO_2 purge from WGS	10
	Stream 13	Water outlet from condenser	13
	Stream 19	Ammonia product (liquid)	19
	Stream 21	Haber Bosch loop purge stream	21
	Stream 26	Impacts and emissions associated with raw material extraction and preparation	26
	Stream 27	Impacts associated with the construction and operation of methane fired heating equipment	27

Process Units Included:

Classification:	Type:	Description:
Primary	SMR 1	First SMR, operating at 60% conversion
	SMR 2	Second SMR, achieving a 96.1% overall efficiency
	WGS Reactor	Conversion of CO to CO_2 through the
	Separation Column	Removes CO_2 from the WGS product stream
	Methanation Reactor	Converts remaining traces of CO and CO_2 back to CH_4 to prevent catalyst poisoning within the downstream HB reactor
	HB Reactor	Production of ammonia with a recycle loop to improve efficiency.
Secondary	HX 1	-
	Compressor 1	-
	HX2	-
	Condenser	-
	Compressor 2	-
	Mixer 1	-
	Mixer 2	-
	Flash Drum	-
	Splitter 1	-
	Compressor 3	-
	HX 3	-

Assumptions:

Aspect:	Assumption(s):

System Boundary	• Ecoinvent datasets assumed to be reflective of the secondary feedstock production (ReCiPe Midpoint (H) characterisation)
	• Electricity generation is handled on-site via a steam turbine fed by process steam from methane combustion
	• Heat is supplied via methane combustion
	  ○ Mol/m3 supplied is evaluated using ideal gas law (5 Bar, 298.15 K)
	  ○ 4.5 GJ / tonne NH_3 heat requirement (German UBA, 2000) [384]
	• CO_2 removal within SMR is achieved using Selexol due to its widespread adoption (European Union Joint Research Council, 2007)
	• US natural gas production data used to estimate BAT, as global averages are not available.
	• Excludes SMR/HB plant construction & decommissioning.
	• Costing data taken from literature for grey ammonia (natural gas fed without CCS) in Asia (S&P Global Commodity Insights, 2023)

Mass balance	• 60% conversion efficiency within primary SMR (European Union Joint Research Council, 2007) • 96.1% conversion efficiency within second SMR (derived from mass balance and primary data for outlet stream composition) (European Union Joint Research Council, 2007) • Steam to methane ratio of 3:1 (European Union Joint Research Council, 2007) • 98% conversion within WGS reactor (European Union Joint Research Council, 2007) • 100% CO & CO_2 conversion efficiency within methanation reactor (D'Angelo, et al., 2021) • Emissions calculations from methane combustion for steam generation assume an optimal 90% combustion efficiency (Mickey, 2017) and 84.3% heat recovery (Najmi & Arhosazni, 2006)
Energy balance	• Average values for BAT plants (29.6 GJ/tonne NH_3) taken from an LCA/TEA with matching system boundaries [384]. This was then sense checked against a consideration of minimum energy required through enthalpy calculations. Energy supplied by methane in SMR reactions is subsequently excluded as impacts are captured by the process' mass balance; this leaves 4500 MJ/FU of heat supplied by natural gas combustion. • Methane energy content of 52 MJ/kg and sourcing from natural gas (fossil) • Energy efficiency of methane burners assumed to be 90% as detailed in literature (Mickey, 2017)
Waste handling	• Gaseous emissions are directly vented.

	• Liquid effluents released to waterways.
Transportation	• Not included
Miscellaneous	• None

Stream Table:

Stream	Species In (kmol/hr)							Species In (kg/hr)							Totals
	CH4	H2O	CO	H2	CO2	N2	NH3	CH4	H2O	CO	H2	CO2	N2	NH3	
1	23.09642168	0	0	0	0	0	0	369.542747	0	0	0	0	0	0	*369.542747*
2	0	69.289265	0	0	0	0	0	0	1247.206771	0	0	0	0	0	*1247.206771*
3	9.238568672	55.431412	13.85785301	41.573559	0	0	0	147.817099	997.7654166	388.019884	83.147118	0	0	0	*1616.749518*
4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	*0.000000*
5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	*0.000000*
6	0.360304178	46.5531475	22.7361175	68.2083525	0	0	0	5.76486685	837.9566557	636.61129	136.416705	0	0	0	*1616.749518*
7	0.360304178	46.5531475	22.7361175	68.2083525	0	0	0	5.76486685	837.9566557	636.61129	136.416705	0	0	0	*1616.749518*
8	0.360304178	24.2717524	0.45472235	90.4897477	22.28139515	0	0	5.76486685	436.891543	12.7322258	180.979495	980.381387	0	0	*1616.749518*
9	0.360304178	24.2717524	0.45472235	90.4897477	22.28139515	0	0	5.76486685	436.891543	12.7322258	180.979495	980.381387	0	0	*1616.749518*
10	0	0	0	0	22.28139515	0	0	0	0	0	0	980.381387	0	0	*980.381387*
11	0.360304178	24.2717524	0.45472235	90.4897477	0	0	0	5.76486685	436.891543	12.7322258	180.979495	0	0	0	*636.368131*
12	0.815026528	24.7264747	0	89.1255806	0	0	0	13.0404245	445.0765453	0	178.251161	0	0	0	*636.368131*
13	0	24.7264747	0	0	0	0	0	0	445.0765453	0	0	0	0	0	*445.076545*
14	0.815026528	0	0	89.1255806	0	0	0	13.0404245	0	0	178.251161	0	0	0	*191.291586*
15	0.815026528	0	0	89.1255806	0	0	0	13.0404245	0	0	178.251161	0	0	0	*191.291586*
16	0	0	0	0	0	29.7364711	0	0	0	0	0	0	832.621191	0	*832.621191*
17	0.815026528	0	0	89.1255806	0	29.7364711	0	13.0404245	0	0	178.251161	0	832.621191	0	*1023.912777*
18	20.34251538	0	0	369.536571	0	108.493132	139.26747	325.480246	0	0	739.073141	0	3037.8077	2367.546998	*6469.908089*
19	0	0	0	0.8412385	0	0.3094244	58.8235294	0	0	0	1.682477	0	8.6638833	1000	*1010.346360*
20	20.34251538	0	0	368.695332	0	108.183708	80.4439411	325.480246	0	0	737.390664	0	3029.14382	1367.546998	*5459.561729*
21	0.815026528	0	0	0.03784118	0	0.0114979	0.00771378	13.0404245	0	0	0.07568236	0	0.3219411	0.131134237	*13.569182*
22	19.52748885	0	0	368.657491	0	108.17221	80.4362273	312.439822	0	0	737.314982	0	3028.82188	1367.415864	*5445.992546*
23	19.52748885	0	0	368.657491	0	108.17221	80.4362273	312.439822	0	0	737.314982	0	3028.82188	1367.415864	*5445.992546*
24	19.52748885	0	0	368.657491	0	108.17221	80.4362273	312.439822	0	0	737.314982	0	3028.82188	1367.415864	*5445.992546*
25	19.52748885	0	0	280.41099	0	78.7566611	139.26747	312.439822	0	0	560.82198	0	2205.18651	2367.546998	*5445.995312*
26	Boundary flow with impacts assessed through Ecoinvent data set: 'natural gas production - US - natural gas, high pressure'														N/A
27	Boundary flow with impacts assessed through Ecoinvent data set: 'natural gas production - US - natural gas, high pressure' & stochiometric evaluation of emissions (CH4 & CO2)														N/A

Lifecycle Assessment (LCA) Data:

Indicator	Value	Unit
Global Warming Potential (GWP)	1998.817114	kg CO_2-eq. / FU
Ozone Depletion	0.000001	kg CFC-11-eq. / FU
Mineral Resource Depletion	1.374034	kg Cu-eq. / FU
Freshwater Eutrophication Potential	0.003315	kg P-eq. / FU
Marine Eutrophication Potential	0.013564	kg N-eq. / FU
Acidification Potential	0.040155	kg SO_2-eq. / FU
Water Use	1.297039	m^3 / FU

Technoeconomic Assessment (TEA) Data:

Variable	Value	Unit
Energy Requirement	26,900	MJ / FU
Total:	26,900	MJ / FU

Variable	Value	Unit
Energy Input	5,000	MJ / FU
Theoretical Energy Requirement	4,500	MJ / FU
Achieved Energy Efficiency	0.9	Decimal
Overall Relative Mass Efficiency:	0.9	Decimal

Variable	Value	Unit
Mass Fed (Total)	2449.37	kg / FU
Mass of Product	1000	kg / FU
Theoretical Maximum Mass Efficiency	0.4157	Decimal
Achieved Mass Efficiency	0.4083	Decimal
Overall Relative Mass Efficiency:	0.982	Decimal

Flow	Price Data	Data Currency	Year	Price 2022£ / FU:	Quantity Req.:	Total Value:	Unit
1 Tonne	655	USD	2023 (Oct)	517.45	1	517.45	£ / FU
					Total:	517.45	£ / FU

Social Impact Assessment (SIA) Data:

Indicator	Sub-Indicator(s)	Sub-Indicator Value(s)	Final Aggregated Indicator Score
Occupational Health and Safety (OSH)	Accidents causing >4 days' absence	0.586213385	0.694329585
	Work-related disease	0.754901847	
	Work-related mortality	0.714012633	
Child Labour	Non-hazardous	0.740585774	0.617058249
	Hazardous		
	Vulnerability	0.493530724	
Forced Labour	Prevalence	0.973555901	0.733543312119765
	Vulnerability	0.493530724	
Access to Electricity	Energy imports, net (% of energy use)	0.849781993	0.491839919
	Fossil fuel energy consumption (% of total)	0.123295692	
	Electric power consumption (kWh per capita)	0.070600891	
	Renewable energy consumption (% of total final energy consumption)	0.1445	
Access to Water	Freshwater withdrawal as % of total	0.791635859	0.679709488
	Water Stress	0.567783117	
Land Use Change	-	0.277838446	0.277838445646095
Utilisation of Hazardous Materials	Deaths caused by dangerous substances per 10,000 workers	0.754900315	0.754900315

Aggregated Final Objective Indicator Scores:

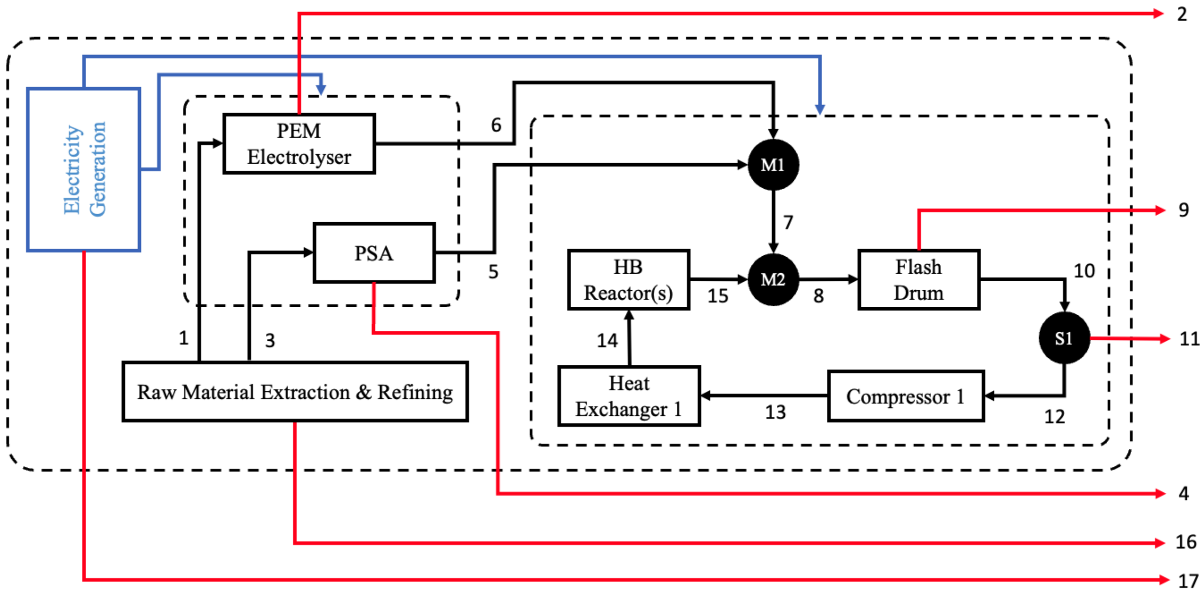
Assessment Strand:	Indicator:	Value:	Units:
LCA	Global Warming Potential (GWP)	1998.817114	kg CO_2-eq. / FU
	Ozone Depletion	0.000001	kg CFC-11-eq. / FU
	Mineral Resource Depletion	1.374034	kg Cu-eq. / FU
	Freshwater Eutrophication Potential	0.003315	kg P-eq. / FU
	Marine Eutrophication Potential	0.013564	kg N-eq. / FU
	Acidification Potential	0.040155	kg SO_2-eq. / FU
	Water Use	1.297039	m^3 / FU
TEA	Energy Demand	26,900	MJ / FU
	Energy Efficiency (%)	0.9	%
	Mass Efficiency (%)	0.982	%
	Est. Purchase Price (2022 £)	517.45	2022 £ / FU
SIA	Occupational Health and Safety (OSH)	0.694329585	-
	Child Labour	0.617058249	-
	Forced Labour	0.733543312	-
	Access to Electricity	0.491839919	-
	Access to Water	0.679709488	-
	Land Use Change	0.277838446	-
	Utilisation of Hazardous Materials	0.754900315	-

Spoke Data Sheet (I.D. 1.3)
(NH_3 from Wind Energy PEM Derived H_2 & Haber Bosch)

Inventory Overview:

Quantity:	Character:
Input or Output?	Input
Reference Flow	1 tonne NH_3 via Proton Exchange Membrane derived H_2 & Haber Bosch
Scope	Cradle-to-Gate
Geographic Region	India
Timeframe	2022

System Boundary Block Flow Diagram (BFD):



Spoke Description:

This cradle-to-grave assessment of ammonia production assesses the coupled use of proton exchange membrane (PEM) electrolysis and the Haber-Bosch process. It is assumed that all process heat (values obtained from literature) is provided through wind energy (50:50 onshore offshore mix). PEM electrolysis and Haber-Bosch models from the literature are identified for use (see table below). The impacts of raw material extraction and preparation for the process are examined using the appropriate Ecoinvent data sets and added to the direct emission associated with process operation.

Spoke Sub-Section	Literature / Models Employed
PEM Electrolysis	[384] (Buttler & Spliethoff, 2018)
Haber-Bosch Process	(Araújo & Skogestad, 2008) (Skogestad, 2004) (Morud & Skogestad, 1998)

Pressure swing adsorption is used for the separation of air as an alternative to the conventional cryogenic separation process. The separation is carried out over a carbon molecular sieve an achieves a purity of 99.9% (Lemcoff, 1999). The oxygen and inerts stream remaining after N_2 separation is vented to the atmosphere.

Proton exchange membrane electrolysis is utilised for the generation of H_2 for the Haber-Bosch feed (*Equation 0-13*). In terms of sustainability and environmental impact, PEM water electrolysis is one of the favourable methods for the conversion of renewable energy to high-purity hydrogen;' exhibiting good efficiency and low temperatures. A conversion efficiency of 60% is observed in deployed units with a pure H_2 outlet stream [384] (Kumar & Himabindu, 2019). However, the operating costs are elevated compared to legacy technologies, resulting in a cost of \$10.30/kg (Kumar & Himabindu, 2019). The unit is fed with water and has a pure (>99.99%) H_2, and O_2 and water outlet streams (Kumar & Himabindu, 2019).

Equation 0-11

$$H_2O \rightarrow H_2 + \frac{1}{2}O_2$$

The H2 mixture is compressed to 196.3 bar, mixed with the recycle stream from the NH3 reactor, and then sent to a flash operating at the same pressure and 42 °C. The liquid outlet, rich in NH3, is sent to a flash unit, reaching an NH3 purity of ~98 mol% at the bottom.

The Haber-Bosch reaction system is modelled as a series of adiabatic plug-flow reactors with a void fraction of 33%, loaded with an iron-based catalyst. The kinetic model of the main reaction was directly adapted from the original reference (Morud & Skogestad, 1998) (Equation 0-5).

Equation 0-12

$$N_2 + 3H_2 \leftrightarrow 2NH_3$$

A nitrogen conversion of 25.3% is achieved inside the reactor. The reactor outlet is then cooled down to 27.1 °C and mixed with the fresh feed. It is then sent to the first flash, separating NH_3 from the remaining compounds and closing the loop.

Boundary Flows:

Classification:	Type:	Description:	Notation:
Input(s)	Raw material extraction	Raw material extraction	
Output(s)	Stream 2	Unreacted water and oxygen waste product from PEM electrolysis	2
	Stream 4	Impacts associated with raw material extraction	4
	Stream 9	Ammonia product (liquid)	9
	Stream 11	Haber Bosch loop purge stream	11
	Stream 16	Impacts and emissions associated with raw material extraction and preparation	16
	Stream 17	Impacts associated with the construction and operation of wind farms	17

Process Units Included:

Classification:	Type:	Description:
Primary	PEM Electrolyser	Performs electrolysis of water utilising a proton exchange membrane. Outlet streams contain water, H_2 and N_2.
	Pressure swing absorber (PSA)	Separates air into constituent components. Nitrogen product utilised for HB.
	HB Reactor	Production of ammonia with a recycle loop to improve efficiency.
Secondary	Mixer 1	-
	Mixer 2	-
	Flash Drum	-
	Compressor 1	-
	Heat Exchanger 1	-

Assumptions:

Aspect:	Assumption(s):
System Boundary	• Air and water are available without burden • Inclusive of onsite wind energy production • Excludes eHB plant construction & decommissioning • Costing data taken from literature for green ammonia in Asia (S&P Global Commodity Insights, 2023)
Mass balance	• 60% efficient PEM electrolyser units [384] • 50% efficient PSA unit (Buttler & Spliethoff, 2018)
Energy balance	• 35.5 GJ/tonne NH_3 for H_2 electrolysis [384] • 2.7 GJ/tonne NH_3 for cryogenic N_2 separation from air and Haber Bosch loop [384]
Waste handling	• Gaseous emissions vented to atmosphere • Liquid emissions discharged to waterways
Transportation	• Not included
Miscellaneous	• None

Stream Table:

Stream	Species In (kmol/hr)					Species In (kg/hr)					Totals
	N2	O2	H2O	H2	NH3	N2	O2	H2O	H2	NH3	
1	0	0	148.5426343	0	0	0	0	2673.76742	0	0	*2673.767418*
2	0	44.5627903	59.41705374	0	0	0	1426.00929	1069.50697	0	0	*2495.516257*
3	59.47294225	16.6962973	0	0	0	1665.24238	534.281514	0	0	0	*2199.523897*
4	29.73647112	16.6962973	0	0	0	832.621191	534.281514	0	0	0	*1366.902705*
5	29.73647112	0	0	0	0	832.621191	0	0	0	0	*832.621191*
6	0	0	0	89.1255806	0	0	0	0	178.2511612	0	*178.251161*
7	29.73647112	0	0	89.1255806	0	832.621191	0	0	178.2511612	0	*1010.872353*
8	108.4931323	0	0	369.536571	139.2674705	3037.8077	0	0	739.0731415	2367.547	*6144.427843*
9	0.309424404	0	0	0.8412385	58.82352941	8.6638833	0	0	1.682477002	1000	*1010.346360*
10	108.1837079	0	0	368.695332	80.44394106	3029.14382	0	0	737.3906645	1367.547	*5134.081483*
11	0.011497896	0	0	0.03784118	0.007713779	0.3219411	0	0	0.075682356	0.13113424	*0.528758*
12	108.17221	0	0	368.657491	80.43622728	3028.82188	0	0	737.3149821	1367.41586	*5133.552725*
13	108.17221	0	0	368.657491	80.43622728	3028.82188	0	0	737.3149821	1367.41586	*5133.552725*
14	108.17221	0	0	368.657491	80.43622728	3028.82188	0	0	737.3149821	1367.41586	*5133.552725*
15	78.75666114	0	0	280.41099	139.2674705	2205.18651	0	0	560.8219803	2367.547	*5133.555490*

Lifecycle Assessment (LCA) Data:

Indicator	Value	Unit
Global Warming Potential (GWP)	271.296214	kg CO_2-eq. / FU
Ozone Depletion	0.000015	kg CFC-11-eq. / FU
Mineral Resource Depletion	199.989961	kg Cu-eq. / FU
Freshwater Eutrophication Potential	0.119691	kg P-eq. / FU
Marine Eutrophication Potential	0.358032	kg N-eq. / FU
Acidification Potential	1.324902	kg SO_2-eq. / FU
Water Use	2.517823	m^3 / FU

Technoeconomic Assessment (TEA) Data

Variable	Value	Unit
Energy Requirement	38,200	MJ / FU
Total:	38,200	MJ / FU

Variable	Value	Unit
Energy Input	38,200	MJ / FU
Theoretical Energy Requirement	38,200	MJ / FU
Achieved Energy Efficiency	1	Decimal
Overall Relative Mass Efficiency:	1	Decimal

Variable	Value	Unit
Mass Fed (Total)	4873.29	kg / FU
Mass of Product	1000	kg / FU
Theoretical Maximum Mass Efficiency	0.3698	Decimal
Achieved Mass Efficiency	0.2052	Decimal
Overall Relative Mass Efficiency:	0.5549	0.982

Flow	Price Data	Data Currency	Year	Price 2022£ / FU:	Quantity Req.:	Total Value:
1 Tonne	781.45	USD	2023 (Oct)	617.35	1	617.35
					Total:	617.35

Social Impact Assessment (SIA) Data:

Indicator	Sub-Indicator(s)	Sub-Indicator Value(s)	Final Aggregated Indicator Score
Occupational Health and Safety (OSH)	Accidents causing >4 days' absence	0.586213385	0.611831817
	Work-related disease	0.754901847	
	Work-related mortality	0.714012633	
Child Labour	Non-hazardous	0.740585774	0.607493035
	Hazardous		
	Vulnerability	0.493530724	
Forced Labour	Prevalence	0.973555901	0.69338248591082
	Vulnerability	0.493530724	
Access to Electricity	Energy imports, net (% of energy use)	0.849781993	0.476854933524488
	Fossil fuel energy consumption (% of total)	0.123295692	
	Electric power consumption (kWh per capita)	0.070600891	
	Renewable energy consumption (% of total final energy consumption)	0.1445	
Access to Water	Freshwater withdrawal as % of total	0.791635859	0.498116751
	Water Stress	0.567783117	
Land Use Change	-	0.277838446	0.194659486476648
Utilisation of Hazardous Materials	Deaths caused by dangerous substances per 10,000 workers	0.754900315	0.591436178275647

Aggregated Final Objective Indicator Scores:

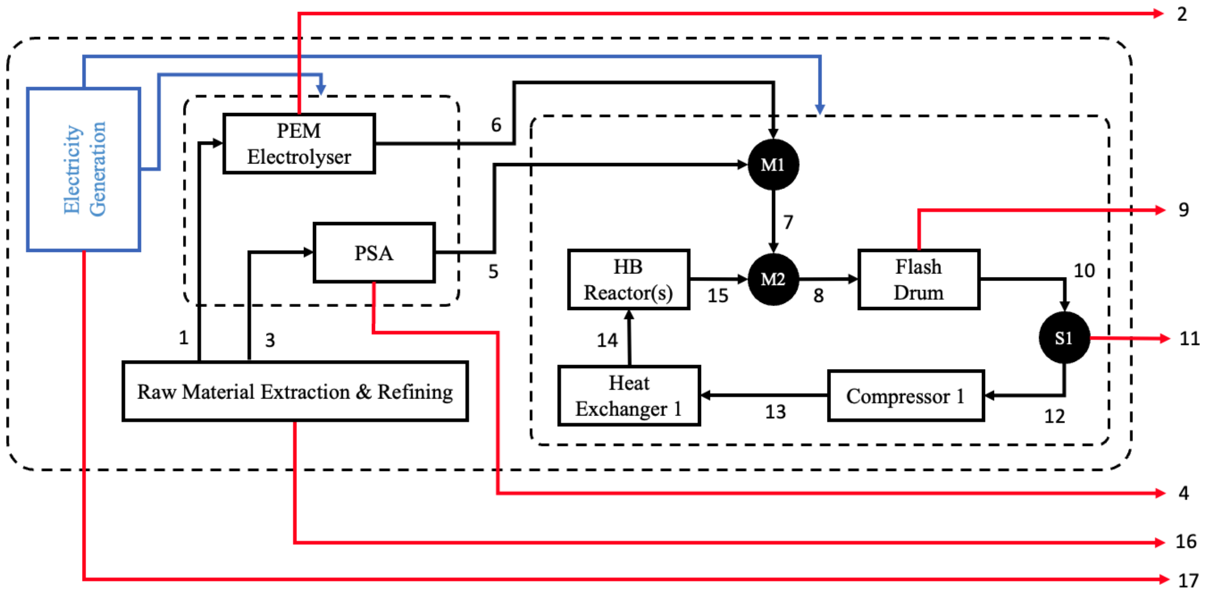
Assessment Strand:	Indicator:	Value:	Units:
LCA	Global Warming Potential (GWP)	271.296214	kg CO_2-eq. / FU
	Ozone Depletion	0.000015	kg CFC-11-eq. / FU
	Mineral Resource Depletion	199.989961	kg Cu-eq. / FU
	Freshwater Eutrophication Potential	0.119691	kg P-eq. / FU
	Marine Eutrophication Potential	0.358032	kg N-eq. / FU
	Acidification Potential	1.324902	kg SO_2-eq. / FU
	Water Use	2.517823	m^3 / FU
TEA	Energy Demand	38,200	MJ / FU
	Energy Efficiency (%)	1	%
	Mass Efficiency (%)	0.5549	%
	Est. Purchase Price (2022 £)	617.35	2022 £ / FU
SIA	Occupational Health and Safety (OSH)	0.611831817	-
	Child Labour	0.607493035	-
	Forced Labour	0.693382486	-
	Access to Electricity	0.476854934	-
	Access to Water	0.498116751	-
	Land Use Change	0.194659486	-
	Utilisation of Hazardous Materials	0.591436178	-

Spoke Data Sheet (I.D. 1.4)
(NH_3 from Wind Energy PEM Derived H_2 & Haber Bosch)

Inventory Overview:

Quantity:	Character:
Input or Output?	Input
Reference Flow	1 tonne NH_3 via Proton Exchange Membrane derived H_2 & Haber Bosch
Scope	Cradle-to-Gate
Geographic Region	China
Timeframe	2022

System Boundary Block Flow Diagram (BFD):



Spoke Description:

This cradle-to-grave assessment of ammonia production assesses the coupled use of proton exchange membrane (PEM) electrolysis and the Haber-Bosch process. It is assumed that all process heat (values obtained from literature) is provided through wind energy (50:50 onshore offshore mix). PEM electrolysis and Haber-Bosch models from the literature are identified for use (see table below). The impacts of raw material extraction and preparation for the process are examined using the appropriate Ecoinvent data sets and added to the direct emission associated with process operation.

Spoke Sub-Section	Literature / Models Employed
PEM Electrolysis	[384] (Buttler & Spliethoff, 2018)
Haber-Bosch Process	(Araújo & Skogestad, 2008) (Skogestad, 2004) (Morud & Skogestad, 1998)

Pressure swing adsorption is used for the separation of air as an alternative to the conventional cryogenic separation process. The separation is carried out over a carbon molecular sieve an achieves a purity of 99.9% (Lemcoff, 1999). The oxygen and inerts stream remaining after N_2 separation is vented to the atmosphere.

Proton exchange membrane electrolysis is utilised for the generation of H_2 for the Haber-Bosch feed (*Equation 0-13*). In terms of sustainability and environmental impact, PEM water electrolysis is one of the favourable methods for the conversion of renewable energy to high-purity hydrogen;' exhibiting good efficiency and low temperatures. A conversion efficiency of 60% is observed in deployed units with a pure H_2 outlet stream [384] (Kumar & Himabindu, 2019). However, the operating costs are elevated compared to legacy technologies, resulting in a cost of $10.30/kg (Kumar & Himabindu, 2019). The unit is fed with water and has a pure (>99.99%) H_2, and O_2 and water outlet streams (Kumar & Himabindu, 2019).

Equation 0-13

$$H_2O \rightarrow H_2 + \frac{1}{2}O_2$$

The H2 mixture is compressed to 196.3 bar, mixed with the recycle stream from the NH3 reactor, and then sent to a flash operating at the same pressure and 42 °C. The liquid outlet, rich in NH3, is sent to a flash unit, reaching an NH3 purity of ~98 mol% at the bottom.

The Haber-Bosch reaction system is modelled as a series of adiabatic plug-flow reactors with a void fraction of 33%, loaded with an iron-based catalyst. The kinetic model of the main reaction was directly adapted from the original reference (Morud & Skogestad, 1998) (Equation 0-5).

Equation 0-14

$$N_2 + 3H_2 \leftrightarrow 2NH_3$$

A nitrogen conversion of 25.3% is achieved inside the reactor. The reactor outlet is then cooled down to 27.1 °C and mixed with the fresh feed. It is then sent to the first flash, separating NH_3 from the remaining compounds and closing the loop.

Boundary Flows:

Classification:	Type:	Description:	Notation:
Input(s)	Raw material extraction	Raw material extraction	
Output(s)	Stream 2	Unreacted water and oxygen waste product from PEM electrolysis	2
	Stream 4	Impacts associated with raw material extraction	4
	Stream 9	Ammonia product (liquid)	9
	Stream 11	Haber Bosch loop purge stream	11
	Stream 16	Impacts and emissions associated with raw material extraction and preparation	16
	Stream 17	Impacts associated with the construction and operation of wind farms	17

Process Units Included:

Classification:	Type:	Description:
Primary	PEM Electrolyser	Performs electrolysis of water utilising a proton exchange membrane. Outlet streams contain water, H_2 and N_2.
	Pressure swing absorber (PSA)	Separates air into constituent components. Nitrogen product utilised for HB.
	HB Reactor	Production of ammonia with a recycle loop to improve efficiency.
Secondary	Mixer 1	-
	Mixer 2	-
	Flash Drum	-
	Compressor 1	-
	Heat Exchanger 1	-

Assumptions:

Aspect:	Assumption(s):
System Boundary	• Air and water are available without burden • Inclusive of onsite wind energy production • Excludes eHB plant construction & decommissioning • Costing data taken from literature for green ammonia in Asia (S&P Global Commodity Insights, 2023)
Mass balance	• 60% efficient PEM electrolyser units [384] • 50% efficient PSA unit (Buttler & Spliethoff, 2018)
Energy balance	• 35.5 GJ/tonne NH_3 for H_2 electrolysis [384] • 2.7 GJ/tonne NH_3 for cryogenic N_2 separation from air and Haber Bosch loop [384]
Waste handling	• Gaseous emissions vented to atmosphere • Liquid emissions discharged to waterways
Transportation	• Not included
Miscellaneous	• None

Stream Table:

Stream	Species In (kmol/hr)					Species In (kg/hr)					Totals
	N2	O2	H2O	H2	NH3	N2	O2	H2O	H2	NH3	
1	0	0	148.5426343	0	0	0	0	2673.76742	0	0	*2673.767418*
2	0	44.5627903	59.41705374	0	0	0	1426.00929	1069.50697	0	0	*2495.516257*
3	59.47294225	16.6962973	0	0	0	1665.24238	534.281514	0	0	0	*2199.523897*
4	29.73647112	16.6962973	0	0	0	832.621191	534.281514	0	0	0	*1366.902705*
5	29.73647112	0	0	0	0	832.621191	0	0	0	0	*832.621191*
6	0	0	0	89.1255806	0	0	0	0	178.2511612	0	*178.251161*
7	29.73647112	0	0	89.1255806	0	832.621191	0	0	178.2511612	0	*1010.872353*
8	108.4931323	0	0	369.536571	139.2674705	3037.8077	0	0	739.0731415	2367.547	*6144.427843*
9	0.309424404	0	0	0.8412385	58.82352941	8.6638833	0	0	1.682477002	1000	*1010.346360*
10	108.1837079	0	0	368.695332	80.44394106	3029.14382	0	0	737.3906645	1367.547	*5134.081483*
11	0.011497896	0	0	0.03784118	0.007713779	0.3219411	0	0	0.075682356	0.13113424	*0.528758*
12	108.17221	0	0	368.657491	80.43622728	3028.82188	0	0	737.3149821	1367.41586	*5133.552725*
13	108.17221	0	0	368.657491	80.43622728	3028.82188	0	0	737.3149821	1367.41586	*5133.552725*
14	108.17221	0	0	368.657491	80.43622728	3028.82188	0	0	737.3149821	1367.41586	*5133.552725*
15	78.75666114	0	0	280.41099	139.2674705	2205.18651	0	0	560.8219803	2367.547	*5133.555490*

Lifecycle Assessment (LCA) Data:

Indicator	Value	Unit
Global Warming Potential (GWP)	271.296214	kg CO_2-eq. / FU
Ozone Depletion	0.000015	kg CFC-11-eq. / FU
Mineral Resource Depletion	199.989961	kg Cu-eq. / FU
Freshwater Eutrophication Potential	0.119691	kg P-eq. / FU
Marine Eutrophication Potential	0.358032	kg N-eq. / FU
Acidification Potential	1.324902	kg SO_2-eq. / FU
Water Use	2.517823	m^3 / FU

Technoeconomic Assessment (TEA) Data

Variable	Value	Unit
Energy Requirement	38,200	MJ / FU
Total:	38,200	MJ / FU

Variable	Value	Unit
Energy Input	38,200	MJ / FU
Theoretical Energy Requirement	38,200	MJ / FU
Achieved Energy Efficiency	1	Decimal
Overall Relative Mass Efficiency:	1	Decimal

Variable	Value	Unit
Mass Fed (Total)	4873.29	kg / FU
Mass of Product	1000	kg / FU
Theoretical Maximum Mass Efficiency	0.3698	Decimal
Achieved Mass Efficiency	0.2052	Decimal
Overall Relative Mass Efficiency:	0.5549	0.982

Flow	Price Data	Data Currency	Year	Price 2022£ / FU:	Quantity Req.:	Total Value:
1 Tonne	781.45	USD	2023 (Oct)	617.35	1	617.35
					Total:	617.35

Social Impact Assessment (SIA) Data:

Indicator	Sub-Indicator(s)	Sub-Indicator Value(s)	Final Aggregated Indicator Score
Occupational Health and Safety (OSH)	Accidents causing >4 days' absence	0.586213385	0.694329585
	Work-related disease	0.754901847	
	Work-related mortality	0.714012633	
Child Labour	Non-hazardous	0.740585774	0.617058249
	Hazardous		
	Vulnerability	0.493530724	
Forced Labour	Prevalence	0.973555901	0.733543312119765
	Vulnerability	0.493530724	
Access to Electricity	Energy imports, net (% of energy use)	0.849781993	0.491839919
	Fossil fuel energy consumption (% of total)	0.123295692	
	Electric power consumption (kWh per capita)	0.070600891	
	Renewable energy consumption (% of total final energy consumption)	0.1445	
Access to Water	Freshwater withdrawal as % of total	0.791635859	0.679709488
	Water Stress	0.567783117	
Land Use Change	-	0.277838446	0.277838445646095
Utilisation of Hazardous Materials	Deaths caused by dangerous substances per 10,000 workers	0.754900315	0.754900315

Aggregated Final Objective Indicator Scores:

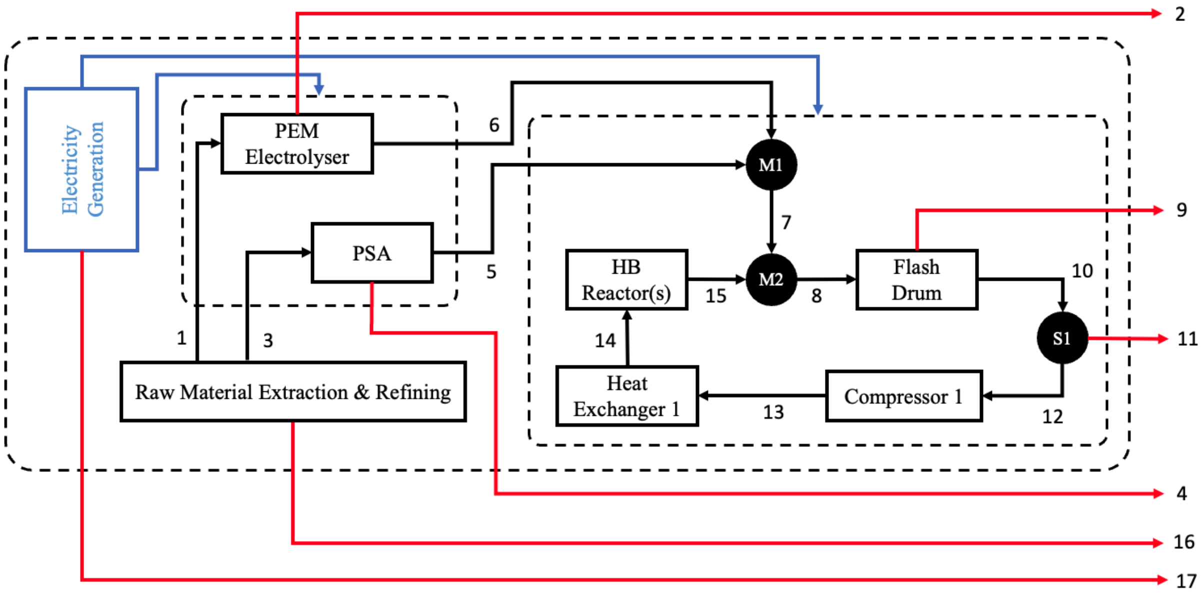
Assessment Strand:	Indicator:	Value:	Units:
LCA	Global Warming Potential (GWP)	271.296214	kg CO_2-eq. / FU
	Ozone Depletion	0.000015	kg CFC-11-eq. / FU
	Mineral Resource Depletion	199.989961	kg Cu-eq. / FU
	Freshwater Eutrophication Potential	0.119691	kg P-eq. / FU
	Marine Eutrophication Potential	0.358032	kg N-eq. / FU
	Acidification Potential	1.324902	kg SO_2-eq. / FU
	Water Use	2.517823	m^3 / FU
TEA	Energy Demand	38,200	MJ / FU
	Energy Efficiency (%)	1	%
	Mass Efficiency (%)	0.5549	%
	Est. Purchase Price (2022 £)	617.35	2022 £ / FU
SIA	Occupational Health and Safety (OSH)	0.694329585	-
	Child Labour	0.617058249	-
	Forced Labour	0.733543312	-
	Access to Electricity	0.491839919	-
	Access to Water	0.679709488	-
	Land Use Change	0.277838446	-
	Utilisation of Hazardous Materials	0.754900315	-

Spoke Data Sheet (I.D. 1.5)
(NH_3 from Grid Energy PEM Derived H_2 & Haber Bosch)

Inventory Overview:

Quantity:	Character:
Input or Output?	Input
Reference Flow	1 tonne NH_3 via Proton Exchange Membrane derived H_2 & Haber Bosch
Scope	Cradle-to-Gate
Geographic Region	India
Timeframe	2022

System Boundary Block Flow Diagram (BFD):



Spoke Description:

This cradle-to-grave assessment of ammonia production assesses the coupled use of proton exchange membrane (PEM) electrolysis and the Haber-Bosch process. It is assumed that all process heat (values obtained from literature) is provided through the grid mix of the examined country. PEM electrolysis and Haber-Bosch models from the literature are identified for use (see table below). The impacts of raw material extraction and preparation for the process are examined using the appropriate Ecoinvent data sets and added to the direct emission associated with process operation.

Spoke Sub-Section	Literature / Models Employed
PEM Electrolysis	[384] (Buttler & Spliethoff, 2018)
Haber-Bosch Process	(Araújo & Skogestad, 2008) (Skogestad, 2004) (Morud & Skogestad, 1998)

Pressure swing adsorption is used for the separation of air as an alternative to the conventional cryogenic separation process. The separation is carried out over a carbon molecular sieve an achieves a purity of 99.9% (Lemcoff, 1999). The oxygen and inerts stream remaining after N_2 separation is vented to the atmosphere.

Proton exchange membrane electrolysis is utilised for the generation of H_2 for the Haber-Bosch feed (*Equation 0-13*). In terms of sustainability and environmental impact, PEM water electrolysis is one of the favourable methods for the conversion of renewable energy to high-purity hydrogen;' exhibiting good efficiency and low temperatures. A conversion efficiency of 60% is observed in deployed units with a pure H_2 outlet stream [384] (Kumar & Himabindu, 2019). However, the operating costs are elevated compared to legacy technologies, resulting in a cost of \$10.30/kg (Kumar & Himabindu, 2019). The unit is fed with water and has a pure (>99.99%) H_2, and O_2 and water outlet streams (Kumar & Himabindu, 2019).

Equation 0-15

$$H_2O \rightarrow H_2 + \frac{1}{2}O_2$$

The H2 mixture is compressed to 196.3 bar, mixed with the recycle stream from the NH3 reactor, and then sent to a flash operating at the same pressure and 42 °C. The liquid outlet, rich in NH3, is sent to a flash unit, reaching an NH3 purity of ~98 mol% at the bottom.

The Haber-Bosch reaction system is modelled as a series of adiabatic plug-flow reactors with a void fraction of 33%, loaded with an iron-based catalyst. The kinetic model of the main reaction was directly adapted from the original reference (Morud & Skogestad, 1998) (Equation 0-5).

Equation 0-16

$$N_2 + 3H_2 \leftrightarrow 2NH_3$$

A nitrogen conversion of 25.3% is achieved inside the reactor. The reactor outlet is then cooled down to 27.1 °C and mixed with the fresh feed. It is then sent to the first flash, separating NH_3 from the remaining compounds and closing the loop.

Boundary Flows:

Classification:	Type:	Description:	Notation:
Input(s)	Raw material extraction	Raw material extraction	
Output(s)	Stream 2	Unreacted water and oxygen waste product from PEM electrolysis	2
	Stream 4	Impacts associated with raw material extraction	4
	Stream 9	Ammonia product (liquid)	9
	Stream 11	Haber Bosch loop purge stream	11
	Stream 16	Impacts and emissions associated with raw material extraction and preparation	16
	Stream 17	Impacts associated with the construction and operation of wind farms	17

Process Units Included:

Classification:	Type:	Description:
Primary	PEM Electrolyser	Performs electrolysis of water utilising a proton exchange membrane. Outlet streams contain water, H_2 and N_2.
	Pressure swing absorber (PSA)	Separates air into constituent components. Nitrogen product utilised for HB.
	HB Reactor	Production of ammonia with a recycle loop to improve efficiency.
Secondary	Mixer 1	-
	Mixer 2	-
	Flash Drum	-
	Compressor 1	-
	Heat Exchanger 1	-

Assumptions:

Aspect:	Assumption(s):
System Boundary	• Air and water are available without burden. • Inclusive of domestic energy production • Excludes eHB plant construction & decommissioning. • Costing data taken from literature for green ammonia in Asia (S&P Global Commodity Insights, 2023), reflecting the process architecture and energy demands.
Mass balance	• 60% efficient PEM electrolyser units [384] • 50% efficient PSA unit (Buttler & Spliethoff, 2018)
Energy balance	• 35.5 GJ/tonne NH_3 for H_2 electrolysis [384] • 2.7 GJ/tonne NH_3 for cryogenic N_2 separation from air and Haber Bosch loop [384]
Waste handling	• Gaseous emissions vented to atmosphere • Liquid emissions discharged to waterways
Transportation	• Not included
Miscellaneous	• None

Stream Table:

Stream	Species In (kmol/hr)					Species In (kg/hr)					Totals
	N2	O2	H2O	H2	NH3	N2	O2	H2O	H2	NH3	
1	0	0	148.5426343	0	0	0	0	2673.76742	0	0	*2673.767418*
2	0	44.5627903	59.41705374	0	0	0	1426.00929	1069.50697	0	0	*2495.516257*
3	59.47294225	16.6962973	0	0	0	1665.24238	534.281514	0	0	0	*2199.523897*
4	29.73647112	16.6962973	0	0	0	832.621191	534.281514	0	0	0	*1366.902705*
5	29.73647112	0	0	0	0	832.621191	0	0	0	0	*832.621191*
6	0	0	0	89.1255806	0	0	0	0	178.2511612	0	*178.251161*
7	29.73647112	0	0	89.1255806	0	832.621191	0	0	178.2511612	0	*1010.872353*
8	108.4931323	0	0	369.536571	139.2674705	3037.8077	0	0	739.0731415	2367.547	*6144.427843*
9	0.309424404	0	0	0.8412385	58.82352941	8.6638833	0	0	1.682477002	1000	*1010.346360*
10	108.1837079	0	0	368.695332	80.44394106	3029.14382	0	0	737.3906645	1367.547	*5134.081483*
11	0.011497896	0	0	0.03784118	0.007713779	0.3219411	0	0	0.075682356	0.13113424	*0.528758*
12	108.17221	0	0	368.657491	80.43622728	3028.82188	0	0	737.3149821	1367.41586	*5133.552725*
13	108.17221	0	0	368.657491	80.43622728	3028.82188	0	0	737.3149821	1367.41586	*5133.552725*
14	108.17221	0	0	368.657491	80.43622728	3028.82188	0	0	737.3149821	1367.41586	*5133.552725*
15	78.75666114	0	0	280.41099	139.2674705	2205.18651	0	0	560.8219803	2367.547	*5133.555490*

Lifecycle Assessment (LCA) Data:

Indicator	Value	Unit
Global Warming Potential (GWP)	9089.246998	kg CO_2-eq. / FU
Ozone Depletion	0.000079	kg CFC-11-eq. / FU
Mineral Resource Depletion	72.770813	kg Cu-eq. / FU
Freshwater Eutrophication Potential	7.848925	kg P-eq. / FU
Marine Eutrophication Potential	12.745240	kg N-eq. / FU
Acidification Potential	71.107075	kg SO_2-eq. / FU
Water Use	39.733154	m^3 / FU

Technoeconomic Assessment (TEA) Data:

Variable	Value	Unit
Energy Requirement	38,200	MJ / FU
Total:	38,200	MJ / FU

Variable	Value	Unit
Energy Input	38,200	MJ / FU
Theoretical Energy Requirement	38,200	MJ / FU
Achieved Energy Efficiency	1	Decimal
Overall Relative Mass Efficiency:	1	Decimal

Variable	Value	Unit
Mass Fed (Total)	4873.291315	kg / FU
Mass of Product	1000	kg / FU
Theoretical Maximum Mass Efficiency	0.369819422	Decimal
Achieved Mass Efficiency	0.205200128	Decimal
Overall Relative Mass Efficiency:	0.554865741	0.982

Flow	Price Data	Data Currency	Year	Price 2022£ / FU:	Quantity Req.:	Total Value:
1 Tonne	781.45	USD	2023 (Oct)	617.35	1	617.35
					Total:	617.35

Social Impact Assessment (SIA) Data:

<table>
<tr><th>Indicator</th><th>Sub-Indicator(s)</th><th>Sub-Indicator Value(s)</th><th>Final Aggregated Indicator Score</th></tr>
<tr><td rowspan="3">Occupational Health and Safety (OSH)</td><td>Accidents causing >4 days' absence</td><td>0.586213385</td><td rowspan="3">0.611831817</td></tr>
<tr><td>Work-related disease</td><td>0.754901847</td></tr>
<tr><td>Work-related mortality</td><td>0.714012633</td></tr>
<tr><td rowspan="3">Child Labour</td><td>Non-hazardous</td><td rowspan="2">0.740585774</td><td rowspan="3">0.607493035</td></tr>
<tr><td>Hazardous</td></tr>
<tr><td>Vulnerability</td><td>0.493530724</td></tr>
<tr><td rowspan="2">Forced Labour</td><td>Prevalence</td><td>0.973555901</td><td rowspan="2">0.69338248591082</td></tr>
<tr><td>Vulnerability</td><td>0.493530724</td></tr>
<tr><td rowspan="4">Access to Electricity</td><td>Energy imports, net (% of energy use)</td><td>0.849781993</td><td rowspan="4">0.476854933524488</td></tr>
<tr><td>Fossil fuel energy consumption (% of total)</td><td>0.123295692</td></tr>
<tr><td>Electric power consumption (kWh per capita)</td><td>0.070600891</td></tr>
<tr><td>Renewable energy consumption (% of total final energy consumption)</td><td>0.1445</td></tr>
<tr><td rowspan="2">Access to Water</td><td>Freshwater withdrawal as % of total</td><td>0.791635859</td><td rowspan="2">0.498116751</td></tr>
<tr><td>Water Stress</td><td>0.567783117</td></tr>
<tr><td>Land Use Change</td><td>-</td><td>0.277838446</td><td>0.194659486476648</td></tr>
<tr><td>Utilisation of Hazardous Materials</td><td>Deaths caused by dangerous substances per 10,000 workers</td><td>0.754900315</td><td>0.591436178275647</td></tr>
</table>

Aggregated Final Objective Indicator Scores:

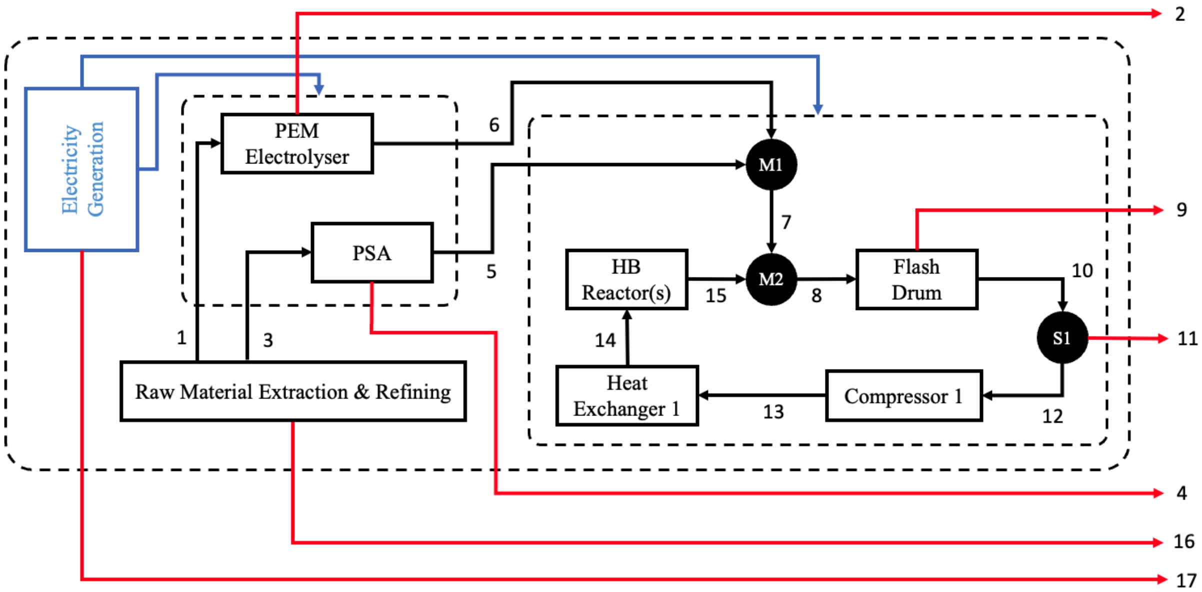
Assessment Strand:	Indicator:	Value:	Units:
LCA	Global Warming Potential (GWP)	9089.246998	kg CO_2-eq. / FU
	Ozone Depletion	0.000079	kg CFC-11-eq. / FU
	Mineral Resource Depletion	72.770813	kg Cu-eq. / FU
	Freshwater Eutrophication Potential	7.848925	kg P-eq. / FU
	Marine Eutrophication Potential	12.745240	kg N-eq. / FU
	Acidification Potential	71.107075	kg SO_2-eq. / FU
	Water Use	39.733154	m^3 / FU
TEA	Energy Demand	38,200	MJ / FU
	Energy Efficiency (%)	1	%
	Mass Efficiency (%)	0.5549	%
	Est. Purchase Price (2022 £)	617.35	2022 £ / FU
SIA	Occupational Health and Safety (OSH)	0.611831817	-
	Child Labour	0.607493035	-
	Forced Labour	0.693382486	-
	Access to Electricity	0.476854934	-
	Access to Water	0.498116751	-
	Land Use Change	0.194659486	-
	Utilisation of Hazardous Materials	0.591436178	-

Spoke Data Sheet (I.D. 1.6)
(NH_3 from Grid Energy PEM Derived H_2 & Haber Bosch)

Inventory Overview:

Quantity:	Character:
Input or Output?	Input
Reference Flow	1 tonne NH_3 via Proton Exchange Membrane derived H_2 & Haber Bosch
Scope	Cradle-to-Gate
Geographic Region	China
Timeframe	2022

System Boundary Block Flow Diagram (BFD):



Spoke Description:

This cradle-to-grave assessment of ammonia production assesses the coupled use of proton exchange membrane (PEM) electrolysis and the Haber-Bosch process. It is assumed that all process heat (values obtained from literature) is provided through the grid mix of the examined country. PEM electrolysis and Haber-Bosch models from the literature are identified for use (see table below). The impacts of raw material extraction and preparation for the process are examined using the appropriate Ecoinvent data sets and added to the direct emission associated with process operation.

Spoke Sub-Section	Literature / Models Employed
PEM Electrolysis	[384] (Buttler & Spliethoff, 2018)
Haber-Bosch Process	(Araújo & Skogestad, 2008) (Skogestad, 2004) (Morud & Skogestad, 1998)

Pressure swing adsorption is used for the separation of air as an alternative to the conventional cryogenic separation process. The separation is carried out over a carbon molecular sieve an achieves a purity of 99.9% (Lemcoff, 1999). The oxygen and inerts stream remaining after N_2 separation is vented to the atmosphere.

Proton exchange membrane electrolysis is utilised for the generation of H_2 for the Haber-Bosch feed (*Equation 0-13*). In terms of sustainability and environmental impact, PEM water electrolysis is one of the favourable methods for the conversion of renewable energy to high-purity hydrogen;' exhibiting good efficiency and low temperatures. A conversion efficiency of 60% is observed in deployed units with a pure H_2 outlet stream [384] (Kumar & Himabindu, 2019). However, the operating costs are elevated compared to legacy technologies, resulting in a cost of $10.30/kg (Kumar & Himabindu, 2019). The unit is fed with water and has a pure (>99.99%) H_2, and O_2 and water outlet streams (Kumar & Himabindu, 2019).

Equation 0-17

$$H_2O \rightarrow H_2 + \frac{1}{2}O_2$$

The H2 mixture is compressed to 196.3 bar, mixed with the recycle stream from the NH3 reactor, and then sent to a flash operating at the same pressure and 42 °C. The liquid outlet, rich in NH3, is sent to a flash unit, reaching an NH3 purity of ~98 mol% at the bottom.

The Haber-Bosch reaction system is modelled as a series of adiabatic plug-flow reactors with a void fraction of 33%, loaded with an iron-based catalyst. The kinetic model of the main reaction was directly adapted from the original reference (Morud & Skogestad, 1998) (Equation 0-5).

Equation 0-18

$$N_2 + 3H_2 \leftrightarrow 2NH_3$$

A nitrogen conversion of 25.3% is achieved inside the reactor. The reactor outlet is then cooled down to 27.1 °C and mixed with the fresh feed. It is then sent to the first flash, separating NH_3 from the remaining compounds and closing the loop.

Boundary Flows:

Classification:	Type:	Description:	Notation:
Input(s)	Raw material extraction	Raw material extraction	
Output(s)	Stream 2	Unreacted water and oxygen waste product from PEM electrolysis	2
	Stream 4	Impacts associated with raw material extraction	4
	Stream 9	Ammonia product (liquid)	9
	Stream 11	Haber Bosch loop purge stream	11
	Stream 16	Impacts and emissions associated with raw material extraction and preparation	16
	Stream 17	Impacts associated with the construction and operation of wind farms	17

Process Units Included:

Classification:	Type:	Description:
Primary	PEM Electrolyser	Performs electrolysis of water utilising a proton exchange membrane. Outlet streams contain water, H_2 and N_2.
	Pressure swing absorber (PSA)	Separates air into constituent components. Nitrogen product utilised for HB.
	HB Reactor	Production of ammonia with a recycle loop to improve efficiency.
Secondary	Mixer 1	-
	Mixer 2	-
	Flash Drum	-
	Compressor 1	-
	Heat Exchanger 1	-

Assumptions:

Aspect:	Assumption(s):
System Boundary	• Air and water are available without burden. • Inclusive of domestic energy production • Excludes eHB plant construction & decommissioning. • Costing data taken from literature for green ammonia in Asia (S&P Global Commodity Insights, 2023), reflecting the process architecture and energy demands.
Mass balance	• 60% efficient PEM electrolyser units [384] • 50% efficient PSA unit (Buttler & Spliethoff, 2018)
Energy balance	• 35.5 GJ/tonne NH_3 for H_2 electrolysis [384] • 2.7 GJ/tonne NH_3 for cryogenic N_2 separation from air and Haber Bosch loop [384]
Waste handling	• Gaseous emissions vented to atmosphere • Liquid emissions discharged to waterways
Transportation	• Not included
Miscellaneous	• None

Stream Table:

Stream	Species In (kmol/hr)					Species In (kg/hr)					Totals
	N2	O2	H2O	H2	NH3	N2	O2	H2O	H2	NH3	
1	0	0	148.5426343	0	0	0	0	2673.76742	0	0	*2673.767418*
2	0	44.5627903	59.41705374	0	0	0	1426.00929	1069.50697	0	0	*2495.516257*
3	59.47294225	16.6962973	0	0	0	1665.24238	534.281514	0	0	0	*2199.523897*
4	29.73647112	16.6962973	0	0	0	832.621191	534.281514	0	0	0	*1366.902705*
5	29.73647112	0	0	0	0	832.621191	0	0	0	0	*832.621191*
6	0	0	0	89.1255806	0	0	0	0	178.2511612	0	*178.251161*
7	29.73647112	0	0	89.1255806	0	832.621191	0	0	178.2511612	0	*1010.872353*
8	108.4931323	0	0	369.536571	139.2674705	3037.8077	0	0	739.0731415	2367.547	*6144.427843*
9	0.309424404	0	0	0.8412385	58.82352941	8.6638833	0	0	1.682477002	1000	*1010.346360*
10	108.1837079	0	0	368.695332	80.44394106	3029.14382	0	0	737.3906645	1367.547	*5134.081483*
11	0.011497896	0	0	0.03784118	0.007713779	0.3219411	0	0	0.075682356	0.13113424	*0.528758*
12	108.17221	0	0	368.657491	80.43622728	3028.82188	0	0	737.3149821	1367.41586	*5133.552725*
13	108.17221	0	0	368.657491	80.43622728	3028.82188	0	0	737.3149821	1367.41586	*5133.552725*
14	108.17221	0	0	368.657491	80.43622728	3028.82188	0	0	737.3149821	1367.41586	*5133.552725*
15	78.75666114	0	0	280.41099	139.2674705	2205.18651	0	0	560.8219803	2367.547	*5133.555490*

Lifecycle Assessment (LCA) Data:

Indicator	Value	Unit
Global Warming Potential (GWP)	9089.246998	kg CO_2-eq. / FU
Ozone Depletion	0.000079	kg CFC-11-eq. / FU
Mineral Resource Depletion	72.770813	kg Cu-eq. / FU
Freshwater Eutrophication Potential	7.848925	kg P-eq. / FU
Marine Eutrophication Potential	12.745240	kg N-eq. / FU
Acidification Potential	71.107075	kg SO_2-eq. / FU
Water Use	39.733154	m^3 / FU

Technoeconomic Assessment (TEA) Data:

Variable	Value	Unit
Energy Requirement	38,200	MJ / FU
Total:	38,200	MJ / FU

Variable	Value	Unit
Energy Input	38,200	MJ / FU
Theoretical Energy Requirement	38,200	MJ / FU
Achieved Energy Efficiency	1	Decimal
Overall Relative Mass Efficiency:	1	Decimal

Variable	Value	Unit
Mass Fed (Total)	4873.291315	kg / FU
Mass of Product	1000	kg / FU
Theoretical Maximum Mass Efficiency	0.369819422	Decimal
Achieved Mass Efficiency	0.205200128	Decimal
Overall Relative Mass Efficiency:	0.554865741	0.982

Flow	Price Data	Data Currency	Year	Price 2022£ / FU:	Quantity Req.:	Total Value:
1 Tonne	781.45	USD	2023 (Oct)	617.35	1	617.35
					Total:	617.35

Social Impact Assessment (SIA) Data:

Indicator	Sub-Indicator(s)	Sub-Indicator Value(s)	Final Aggregated Indicator Score
Occupational Health and Safety (OSH)	Accidents causing >4 days' absence	0.586213385	0.694329585
	Work-related disease	0.754901847	
	Work-related mortality	0.714012633	
Child Labour	Non-hazardous	0.740585774	0.617058249
	Hazardous		
	Vulnerability	0.493530724	
Forced Labour	Prevalence	0.973555901	0.733543312119765
	Vulnerability	0.493530724	
Access to Electricity	Energy imports, net (% of energy use)	0.849781993	0.491839919
	Fossil fuel energy consumption (% of total)	0.123295692	
	Electric power consumption (kWh per capita)	0.070600891	
	Renewable energy consumption (% of total final energy consumption)	0.1445	
Access to Water	Freshwater withdrawal as % of total	0.791635859	0.679709488
	Water Stress	0.567783117	
Land Use Change	-	0.277838446	0.277838445646095
Utilisation of Hazardous Materials	Deaths caused by dangerous substances per 10,000 workers	0.754900315	0.754900315

Aggregated Final Objective Indicator Scores:

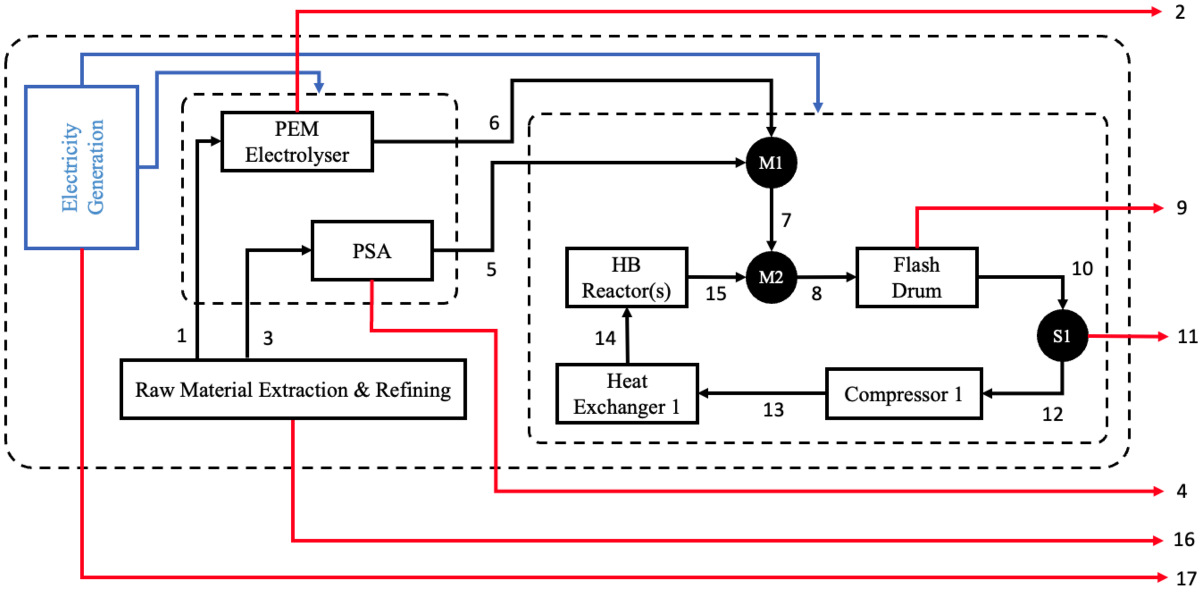
Assessment Strand:	Indicator:	Value:	Units:
LCA	Global Warming Potential (GWP)	7746.435456	kg CO_2-eq. / FU
	Ozone Depletion	0.000072	kg CFC-11-eq. / FU
	Mineral Resource Depletion	78.136307	kg Cu-eq. / FU
	Freshwater Eutrophication Potential	7.176621	kg P-eq. / FU
	Marine Eutrophication Potential	10.922532	kg N-eq. / FU
	Acidification Potential	60.539393	kg SO_2-eq. / FU
	Water Use	34.917053	m^3 / FU
TEA	Energy Demand	38,200	MJ / FU
	Energy Efficiency (%)	1	%
	Mass Efficiency (%)	0.5549	%
	Est. Purchase Price (2022 £)	617.35	2022 £ / FU
SIA	Occupational Health and Safety (OSH)	0.305670415	-
	Child Labour	0.617058249	-
	Forced Labour	0.733543312	-
	Access to Electricity	0.491839919	-
	Access to Water	0.679709488	-
	Land Use Change	0.277838446	-
	Utilisation of Hazardous Materials	0.754900315	-

Spoke Data Sheet (I.D. 1.7)
(NH_3 from Grid Energy PEM Derived H_2 & Haber Bosch)

Inventory Overview:

Quantity:	Character:
Input or Output?	Input
Reference Flow	1 tonne NH_3 via Proton Exchange Membrane derived H_2 & Haber Bosch
Scope	Cradle-to-Gate
Geographic Region	Germany
Timeframe	2022

System Boundary Block Flow Diagram (BFD):



Spoke Description:

This cradle-to-grave assessment of ammonia production assesses the coupled use of proton exchange membrane (PEM) electrolysis and the Haber-Bosch process. It is assumed that all process heat (values obtained from literature) is provided through the grid mix of the examined country. PEM electrolysis and Haber-Bosch models from the literature are identified for use (see table below). The impacts of raw material extraction and preparation for the process are examined using the appropriate Ecoinvent data sets and added to the direct emission associated with process operation.

Spoke Sub-Section	Literature / Models Employed
PEM Electrolysis	[384] (Buttler & Spliethoff, 2018)
Haber-Bosch Process	(Araújo & Skogestad, 2008) (Skogestad, 2004) (Morud & Skogestad, 1998)

Pressure swing adsorption is used for the separation of air as an alternative to the conventional cryogenic separation process. The separation is carried out over a carbon molecular sieve an achieves a purity of 99.9% (Lemcoff, 1999). The oxygen and inerts stream remaining after N_2 separation is vented to the atmosphere.

Proton exchange membrane electrolysis is utilised for the generation of H_2 for the Haber-Bosch feed (*Equation 0-13*). In terms of sustainability and environmental impact, PEM water electrolysis is one of the favourable methods for the conversion of renewable energy to high-purity hydrogen;' exhibiting good efficiency and low temperatures. A conversion efficiency of 60% is observed in deployed units with a pure H_2 outlet stream [384] (Kumar & Himabindu, 2019). However, the operating costs are elevated compared to legacy technologies, resulting in a cost of \$10.30/kg (Kumar & Himabindu, 2019). The unit is fed with water and has a pure (>99.99%) H_2, and O_2 and water outlet streams (Kumar & Himabindu, 2019).

Equation 0-19

$$H_2O \rightarrow H_2 + \frac{1}{2}O_2$$

The H2 mixture is compressed to 196.3 bar, mixed with the recycle stream from the NH3 reactor, and then sent to a flash operating at the same pressure and 42 °C. The liquid outlet, rich in NH3, is sent to a flash unit, reaching an NH3 purity of ~98 mol% at the bottom.

The Haber-Bosch reaction system is modelled as a series of adiabatic plug-flow reactors with a void fraction of 33%, loaded with an iron-based catalyst. The kinetic model of the main reaction was directly adapted from the original reference (Morud & Skogestad, 1998) (Equation 0-5).

Equation 0-20

$$N_2 + 3H_2 \leftrightarrow 2NH_3$$

A nitrogen conversion of 25.3% is achieved inside the reactor. The reactor outlet is then cooled down to 27.1 °C and mixed with the fresh feed. It is then sent to the first flash, separating NH_3 from the remaining compounds and closing the loop.

Boundary Flows:

Classification:	Type:	Description:	Notation:
Input(s)	Raw material extraction	Raw material extraction	
Output(s)	Stream 2	Unreacted water and oxygen waste product from PEM electrolysis	2
	Stream 4	Impacts associated with raw material extraction	4
	Stream 9	Ammonia product (liquid)	9
	Stream 11	Haber Bosch loop purge stream	11
	Stream 16	Impacts and emissions associated with raw material extraction and preparation	16
	Stream 17	Impacts associated with the construction and operation of wind farms	17

Process Units Included:

Classification:	Type:	Description:
Primary	PEM Electrolyser	Performs electrolysis of water utilising a proton exchange membrane. Outlet streams contain water, H_2 and N_2.
	Pressure swing absorber (PSA)	Separates air into constituent components. Nitrogen product utilised for HB.
	HB Reactor	Production of ammonia with a recycle loop to improve efficiency.
Secondary	Mixer 1	-
	Mixer 2	-
	Flash Drum	-
	Compressor 1	-
	Heat Exchanger 1	-

Assumptions:

Aspect:	Assumption(s):
System Boundary	• Air and water are available without burden. • Inclusive of domestic energy production • Excludes eHB plant construction & decommissioning. • Costing data taken from literature for green ammonia in Northern Europe (S&P Global Commodity Insights, 2023), reflecting the process architecture and energy demands.
Mass balance	• 60% efficient PEM electrolyser units [384] • 50% efficient PSA unit (Buttler & Spliethoff, 2018)
Energy balance	• 35.5 GJ/tonne NH_3 for H_2 electrolysis [384] • 2.7 GJ/tonne NH_3 for cryogenic N_2 separation from air and Haber Bosch loop [384]
Waste handling	• Gaseous emissions vented to atmosphere • Liquid emissions discharged to waterways
Transportation	• Not included
Miscellaneous	• None

Stream Table:

Stream	Species In (kmol/hr)					Species In (kg/hr)					Totals
	N2	O2	H2O	H2	NH3	N2	O2	H2O	H2	NH3	
1	0	0	148.5426343	0	0	0	0	2673.76742	0	0	*2673.767418*
2	0	44.5627903	59.41705374	0	0	0	1426.00929	1069.50697	0	0	*2495.516257*
3	59.47294225	16.6962973	0	0	0	1665.24238	534.281514	0	0	0	*2199.523897*
4	29.73647112	16.6962973	0	0	0	832.621191	534.281514	0	0	0	*1366.902705*
5	29.73647112	0	0	0	0	832.621191	0	0	0	0	*832.621191*
6	0	0	0	89.1255806	0	0	0	0	178.2511612	0	*178.251161*
7	29.73647112	0	0	89.1255806	0	832.621191	0	0	178.2511612	0	*1010.872353*
8	108.4931323	0	0	369.536571	139.2674705	3037.8077	0	0	739.0731415	2367.547	*6144.427843*
9	0.309424404	0	0	0.8412385	58.82352941	8.6638833	0	0	1.682477002	1000	*1010.346360*
10	108.1837079	0	0	368.695332	80.44394106	3029.14382	0	0	737.3906645	1367.547	*5134.081483*
11	0.011497896	0	0	0.03784118	0.007713779	0.3219411	0	0	0.075682356	0.13113424	*0.528758*
12	108.17221	0	0	368.657491	80.43622728	3028.82188	0	0	737.3149821	1367.41586	*5133.552725*
13	108.17221	0	0	368.657491	80.43622728	3028.82188	0	0	737.3149821	1367.41586	*5133.552725*
14	108.17221	0	0	368.657491	80.43622728	3028.82188	0	0	737.3149821	1367.41586	*5133.552725*
15	78.75666114	0	0	280.41099	139.2674705	2205.18651	0	0	560.8219803	2367.547	*5133.555490*

Lifecycle Assessment (LCA) Data:

Indicator	Value	Unit
Global Warming Potential (GWP)	4950.130655	kg CO_2-eq. / FU
Ozone Depletion	0.000389	kg CFC-11-eq. / FU
Mineral Resource Depletion	118.038974	kg Cu-eq. / FU
Freshwater Eutrophication Potential	5.201067	kg P-eq. / FU
Marine Eutrophication Potential	6.983101	kg N-eq. / FU
Acidification Potential	33.566983	kg SO_2-eq. / FU
Water Use	23.342532	m^3 / FU

Technoeconomic Assessment (TEA) Data:

Variable	Value	Unit
Energy Requirement	38,200	MJ / FU
Total:	38,200	MJ / FU

Variable	Value	Unit
Energy Input	38,200	MJ / FU
Theoretical Energy Requirement	38,200	MJ / FU
Achieved Energy Efficiency	1	Decimal
Overall Relative Mass Efficiency:	1	Decimal

Variable	Value	Unit
Mass Fed (Total)	4873.291315	kg / FU
Mass of Product	1000	kg / FU
Theoretical Maximum Mass Efficiency	0.369819422	Decimal
Achieved Mass Efficiency	0.205200128	Decimal
Overall Relative Mass Efficiency:	0.554865741	0.982

Flow	Price Data	Data Currency	Year	Price 2022£ / FU:	Quantity Req.:	Total Value:
1 Tonne	756.36	USD	2023 (Oct)	597.52	1	597.52
					Total:	597.52

Social Impact Assessment (SIA) Data:

Indicator	Sub-Indicator(s)	Sub-Indicator Value(s)	Final Aggregated Indicator Score
Occupational Health and Safety (OSH)	Accidents causing >4 days' absence	0.929700422	0.704720447
	Work-related disease	0.613791293	
	Work-related mortality	0.640351009	
Child Labour	Non-hazardous	0.90376569	0.899666513
	Hazardous		
	Vulnerability	0.895567336	
Forced Labour	Prevalence	0.980493285	0.938030311
	Vulnerability	0.895567336	
Access to Electricity	Energy imports, net (% of energy use)	0.385998306	0.288767776
	Fossil fuel energy consumption (% of total)	0.211374489	
	Electric power consumption (kWh per capita)	0.127761537	
	Renewable energy consumption (% of total final energy consumption)	0.1717	
Access to Water	Freshwater withdrawal as % of total	0.841279221	0.753130016
	Water Stress	0.664980811	
Land Use Change	-	0.245190502	0.245190502
Utilisation of Hazardous Materials	Deaths caused by dangerous substances per 10,000 workers	0.613788717	0.613788717

Aggregated Final Objective Indicator Scores:

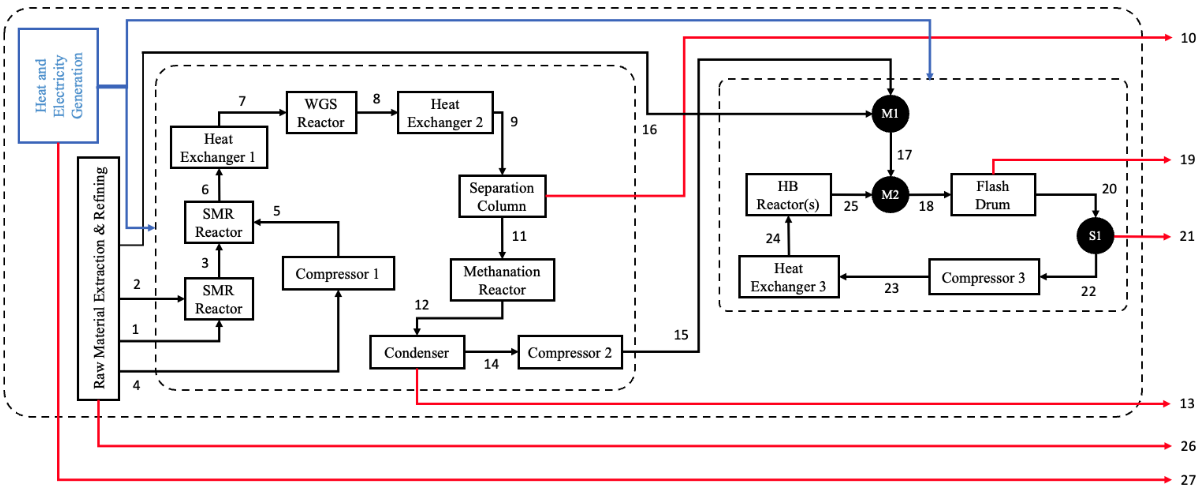
Assessment Strand:	Indicator:	Value:	Units:
LCA	Global Warming Potential (GWP)	4950.130655	kg CO_2-eq. / FU
	Ozone Depletion	0.000389	kg CFC-11-eq. / FU
	Mineral Resource Depletion	118.038974	kg Cu-eq. / FU
	Freshwater Eutrophication Potential	5.201067	kg P-eq. / FU
	Marine Eutrophication Potential	6.983101	kg N-eq. / FU
	Acidification Potential	33.566983	kg SO_2-eq. / FU
	Water Use	23.342532	m^3 / FU
TEA	Energy Demand	38,200	MJ / FU
	Energy Efficiency (%)	1	%
	Mass Efficiency (%)	0.5549	%
	Est. Purchase Price (2022 £)	597.52	2022 £ / FU
SIA	Occupational Health and Safety (OSH)	0.704720447	-
	Child Labour	0.899666513	-
	Forced Labour	0.938030311	-
	Access to Electricity	0.288767776	-
	Access to Water	0.753130016	-
	Land Use Change	0.245190502	-
	Utilisation of Hazardous Materials	0.613788717	-

Spoke Data Sheet (I.D. 1.8)
(NH_3 from Biogas fed Steam Methane Reformation & Haber Bosch)

Inventory Overview:

Quantity:	Character:
Input or Output?	Input
Reference Flow	1 tonne NH_3 via biogas fed Steam Methane Reformation & Haber Bosch
Scope	Cradle-to-Gate
Geographic Region	India
Timeframe	2022

System Boundary Block Flow Diagram (BFD):



Spoke Description:

This cradle-to-grave assessment of ammonia production assesses the coupled use of biomethane fed steam methane reforming and the Haber-Bosch process. It is assumed that all process heat (values obtained from literature) is provided through the combustion of biomethane. Steam methane reformation and Haber-Bosch models from the literature are identified for use (see table below). The impacts of raw material extraction and preparation for the process are examined using the appropriate Ecoinvent data sets reflecting the generation of biogas through the anaerobic digestion of biowaste and its subsequent treatment to produce biomethane. Beyond the biomethane feed, the SMR HB process model remains the same as the natural gas fed datasets. Biowaste is assumed to be procured sans burdens, and the biogenic carbon released through the combustion and reaction of biomethane is take as a zero burden in terms of impact indicators.

Spoke Sub-Section	Literature / Models Employed
Steam Methane Reformation	(D'Angelo, et al., 2021) (Boero, et al., 2021) (European Union Joint Research Council, 2007) (Van Herwijnen, et al., 1973)
Haber-Bosch Process	(Araújo & Skogestad, 2008) (Skogestad, 2004) (Morud & Skogestad, 1998)

In the first modelled step, hydrogen is produced from methane and, in the second, ammonia is synthesised via the Haber–Bosch reaction. Hydrogen is produced by primary and secondary steam methane reforming reactors (SMR) (Equation C-1). The first SMR reactor operates at around 850–900°C and 25–35 bar with the energy required for the endothermic reaction being provided by the combustion of methane. The second SMR reactor is autothermal, air is compressed and fed to the reactor to provide heat of reaction by partial oxidation of the reagents at 900–1000°C.

Equation 0-21

$$CH_4 + H_2O \leftrightarrow CO + 3H_2O$$

The SMR outlet mixture of carbon monoxide, hydrogen, and unreacted steam and methane are introduced into the two-stage water–gas shift (WGS) reactor to maximise CO conversion to hydrogen. The WGS reaction is exothermic, and heat must be removed to minimise CO concentration at equilibrium.

Equation 0-22

$$CO + H_2O \leftrightarrow CO_2 + H_2$$

The residual CO and CO2 in the H2-nitrogen mixture must be removed since they poison the HB catalyst.4 Hence, a methanation unit was placed after the MEA absorber to convert the residual CO and CO2 to methane and water. The vapour outlet of the absorption column is heated to 230 °C and fed to the methanation unit, which is modelled as a plug flow reactor implementing Equation C-3 & Equation C-4.

The residual methane present accumulates in the downstream synthesis loop (argon is also present but not modelled due to its presence in negligible mole fractions and removal in a purge stream).

Equation 0-23

$$CO + 3H_2 \leftrightarrow CH_4 + H_2O$$

Equation 0-24

$$CO_2 + 4H_2 \leftrightarrow CH_4 + 2H_2O$$

Although the steam methane reforming reactions are endothermic, the high reaction temperature and the need to cool substantially for the water gas shift reaction means that there is substantial waste heat available. This heat is used for raising high-pressure steam, which is expanded in steam turbines for compression, mainly used for compression of the feed in the Haber Bosch loop and the reformer combustion air compressor, which are the largest two energy users. The use of methane as feedstock inevitably leads to significant CO2 emissions from the process, and this is further compounded by the use of methane as fuel for the primary reformer furnace. The reaction kinetics are reported in Herwijnen et al. (1973), At the selected operating pressure, the conversion of CO2 and CO is 100%.

The H2 mixture is compressed to 196.3 bar, mixed with the recycle stream from the NH3 reactor, and then sent to a flash operating at the same pressure and 42 °C. The liquid outlet, rich in NH3, is sent to a flash unit, reaching an NH3 purity of ~98 mol% at the bottom.

The Haber-Bosch reaction system is modelled as a series of adiabatic plug-flow reactors with a void fraction of 33%, loaded with an iron-based catalyst. The kinetic model of the main reaction was directly adapted from the original reference (Morud & Skogestad, 1998) (Equation 0-5).

Equation 0-25

$$N_2 + 3H_2 \leftrightarrow 2NH_3$$

A nitrogen conversion of 25.3% is achieved inside the reactor. The reactor outlet is then cooled down to 27.1 °C and mixed with the fresh feed. It is then sent to the first flash, separating NH_3 from the remaining compounds and closing the loop.

Boundary Flows:

Classification:	Type:	Description:	Notation:
Input(s)	Raw material extraction	Ecoinvent used to evaluate the impact of feedstock extraction from the environment	N/A
Output(s)	Stream 10	CO_2 purge from WGS	10
	Stream 13	Water outlet from condenser	13
	Stream 19	Ammonia product (liquid)	19
	Stream 21	Haber Bosch loop purge stream	21
	Stream 26	Impacts and emissions associated with raw material extraction and preparation	26
	Stream 27	Impacts associated with the construction and operation of methane fired heating equipment	27

Process Units Included:

Classification:	Type:	Description:
Primary	SMR 1	First SMR, operating at 60% conversion
	SMR 2	Second SMR, achieving a 96.1% overall efficiency
	WGS Reactor	Conversion of CO to CO_2 through the
	Separation Column	Removes CO_2 from the WGS product stream
	Methanation Reactor	Converts remaining traces of CO and CO_2 back to CH_4 to prevent catalyst poisoning within the downstream HB reactor
	HB Reactor	Production of ammonia with a recycle loop to improve efficiency.
Secondary	HX 1	-
	Compressor 1	-
	HX2	-
	Condenser	-
	Compressor 2	-
	Mixer 1	-
	Mixer 2	-
	Flash Drum	-
	Splitter 1	-
	Compressor 3	-
	HX 3	-

Assumptions:

Aspect:	Assumption(s):
System Boundary	• Ecoinvent datasets assumed to be reflective of the secondary feedstock production (ReCiPe Midpoint (H) characterisation) • Electricity generation is handled on-site via a steam turbine fed by process steam from biomethane combustion • Heat is supplied via biomethane combustion ○ Mol/m3 supplied is evaluated using ideal gas law (5 Bar, 298.15 K) ○ 4.5 GJ / tonne NH_3 heat requirement (German UBA, 2000) [384] • CO_2 removal within SMR is achieved using Selexol due to its widespread adoption (European Union Joint Research Council, 2007) • Biomethane production from biowaste via anaerobic digestion and pressure swing absorption is as modelled as the CH_4 feedstock. • Excludes SMR/HB plant construction & decommissioning • Costing data taken from literature for green ammonia (natural gas fed without CCS) in Asia (S&P Global Commodity Insights, 2023)
Mass balance	• 60% conversion efficiency within primary SMR (European Union Joint Research Council, 2007) • 96.1% conversion efficiency within second SMR (derived from mass balance and primary data for outlet stream composition) (European Union Joint Research Council, 2007) • Steam to methane ratio of 3:1 (European Union Joint Research Council, 2007) • 98% conversion within WGS reactor (European Union Joint Research Council, 2007) • 100% CO & CO_2 conversion efficiency within the methanation reactor (D'Angelo, et al., 2021) • Methane combustion for steam generation assumes an optimal 90% combustion efficiency (Mickey, 2017) and 84.3% heat recovery (Najmi & Arhosazni, 2006)
Energy balance	• Average values for BAT plants (29.6 GJ/tonne NH_3) taken from an LCA/TEA with matching system boundaries [384]. This was then sense checked against a consideration of minimum energy required through enthalpy calculations. Energy supplied by menthane in SMR reactions is subsequently excluded as impacts are captured by the process' mass balance. • Methane energy content of 52 MJ/kg and sourcing from biowaste • Energy efficiency of methane burners assumed to be 90% as detailed in literature (Mickey, 2017)
Waste handling	• Gaseous emissions are directly vented.

	• Liquid effluents released to waterways.
Transportation	• Not included
Miscellaneous	• None

Stream Table:

Stream	Species In (kmol/hr)							Species In (kg/hr)							Totals
	CH4	H2O	CO	H2	CO2	N2	NH3	CH4	H2O	CO	H2	CO2	N2	NH3	
1	23.09642168	0	0	0	0	0	0	369.542747	0	0	0	0	0	0	*369.542747*
2	0	69.289265	0	0	0	0	0	0	1247.206771	0	0	0	0	0	*1247.206771*
3	9.238568672	55.431412	13.85785301	41.573559	0	0	0	147.817099	997.7654166	388.019884	83.147118	0	0	0	*1616.749518*
4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	*0.000000*
5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	*0.000000*
6	0.360304178	46.5531475	22.7361175	68.2083525	0	0	0	5.76486685	837.9566557	636.61129	136.416705	0	0	0	*1616.749518*
7	0.360304178	46.5531475	22.7361175	68.2083525	0	0	0	5.76486685	837.9566557	636.61129	136.416705	0	0	0	*1616.749518*
8	0.360304178	24.2717524	0.45472235	90.4897477	22.28139515	0	0	5.76486685	436.891543	12.7322258	180.979495	980.381387	0	0	*1616.749518*
9	0.360304178	24.2717524	0.45472235	90.4897477	22.28139515	0	0	5.76486685	436.891543	12.7322258	180.979495	980.381387	0	0	*1616.749518*
10	0	0	0	0	22.28139515	0	0	0	0	0	0	980.381387	0	0	*980.381387*
11	0.360304178	24.2717524	0.45472235	90.4897477	0	0	0	5.76486685	436.891543	12.7322258	180.979495	0	0	0	*636.368131*
12	0.815026528	24.7264747	0	89.1255806	0	0	0	13.0404245	445.0765453	0	178.251161	0	0	0	*636.368131*
13	0	24.7264747	0	0	0	0	0	0	445.0765453	0	0	0	0	0	*445.076545*
14	0.815026528	0	0	89.1255806	0	0	0	13.0404245	0	0	178.251161	0	0	0	*191.291586*
15	0.815026528	0	0	89.1255806	0	0	0	13.0404245	0	0	178.251161	0	0	0	*191.291586*
16	0	0	0	0	0	29.7364711	0	0	0	0	0	0	832.621191	0	*832.621191*
17	0.815026528	0	0	89.1255806	0	29.7364711	0	13.0404245	0	0	178.251161	0	832.621191	0	*1023.912777*
18	20.34251538	0	0	369.536571	0	108.493132	139.26747	325.480246	0	0	739.073141	0	3037.8077	2367.546998	*6469.908089*
19	0	0	0	0.8412385	0	0.3094244	58.8235294	0	0	0	1.682477	0	8.6638833	1000	*1010.346360*
20	20.34251538	0	0	368.695332	0	108.183708	80.4439411	325.480246	0	0	737.390664	0	3029.14382	1367.546998	*5459.561729*
21	0.815026528	0	0	0.03784118	0	0.0114979	0.00771378	13.0404245	0	0	0.07568236	0	0.3219411	0.131134237	*13.569182*
22	19.52748885	0	0	368.657491	0	108.17221	80.4362273	312.439822	0	0	737.314982	0	3028.82188	1367.415864	*5445.992546*
23	19.52748885	0	0	368.657491	0	108.17221	80.4362273	312.439822	0	0	737.314982	0	3028.82188	1367.415864	*5445.992546*
24	19.52748885	0	0	368.657491	0	108.17221	80.4362273	312.439822	0	0	737.314982	0	3028.82188	1367.415864	*5445.992546*
25	19.52748885	0	0	280.41099	0	78.7566611	139.26747	312.439822	0	0	560.82198	0	2205.18651	2367.546998	*5445.995312*
26	Boundary flow with impacts assessed through Ecoinvent data sets: ‘treatment of biowaste by anaerobic digestion - RoW – biogas’ & biogas purification to biomethane by pressure swing adsorption - RoW - biomethane, high pressure’														N/A
27	Boundary flow with impacts assessed through Ecoinvent data set: treatment of biowaste by anaerobic digestion - RoW – biogas’ & biogas purification to biomethane by pressure swing adsorption - RoW - biomethane, high pressure’ & stochiometric evaluation of emissions (CH4 & CO2) excluding biogenic carbon														N/A

Lifecycle Assessment (LCA) Data:

Indicator	Value	Unit
Global Warming Potential (GWP)	63.376654	kg CO_2-eq. / FU
Ozone Depletion	0.000001	kg CFC-11-eq. / FU
Mineral Resource Depletion	1.781505	kg Cu-eq. / FU
Freshwater Eutrophication Potential	0.013813	kg P-eq. / FU
Marine Eutrophication Potential	0.027154	kg N-eq. / FU
Acidification Potential	0.137608	kg SO_2-eq. / FU
Water Use	0.110454	m^3 / FU

Technoeconomic Assessment (TEA) Data:

Variable	Value	Unit
Energy Requirement	26,900	MJ / FU
Total:	26,900	MJ / FU

Variable	Value	Unit
Energy Input	5,000	MJ / FU
Theoretical Energy Requirement	4,500	MJ / FU
Achieved Energy Efficiency	0.9	Decimal
Overall Relative Mass Efficiency:	0.9	Decimal

Variable	Value	Unit
Mass Fed (Total)	2449.37	kg / FU
Mass of Product	1000	kg / FU
Theoretical Maximum Mass Efficiency	0.4157	Decimal
Achieved Mass Efficiency	0.4083	Decimal
Overall Relative Mass Efficiency:	0.982	Decimal

Flow	Price Data	Data Currency	Year	Price 2022£ / FU:	Quantity Req.:	Total Value:	Unit
1 Tonne	781.45	USD	2023 (Oct)	617.35	1	617.35	£ / FU
					Total:	617.35	£ / FU

Social Impact Assessment (SIA) Data:

Indicator	Sub-Indicator(s)	Sub-Indicator Value(s)	Final Aggregated Indicator Score
Occupational Health and Safety (OSH)	Accidents causing >4 days' absence	0.586213385	0.611831817
	Work-related disease	0.754901847	
	Work-related mortality	0.714012633	
Child Labour	Non-hazardous	0.740585774	0.607493035
	Hazardous		
	Vulnerability	0.493530724	
Forced Labour	Prevalence	0.973555901	0.69338248591082
	Vulnerability	0.493530724	
Access to Electricity	Energy imports, net (% of energy use)	0.849781993	0.476854933524488
	Fossil fuel energy consumption (% of total)	0.123295692	
	Electric power consumption (kWh per capita)	0.070600891	
	Renewable energy consumption (% of total final energy consumption)	0.1445	
Access to Water	Freshwater withdrawal as % of total	0.791635859	0.498116751
	Water Stress	0.567783117	
Land Use Change	-	0.277838446	0.194659486476648
Utilisation of Hazardous Materials	Deaths caused by dangerous substances per 10,000 workers	0.754900315	0.591436178275647

Aggregated Final Objective Indicator Scores:

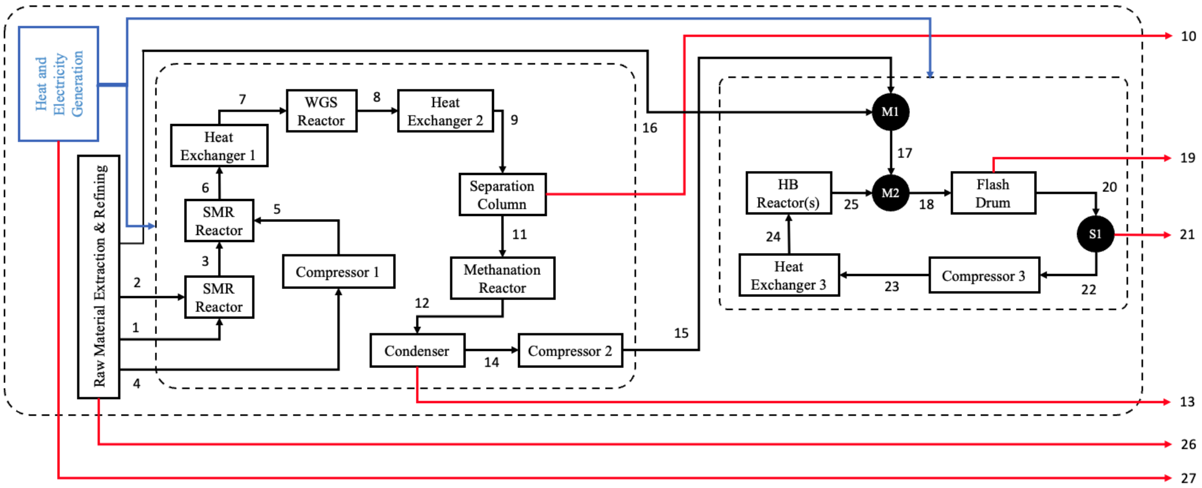
Assessment Strand:	Indicator:	Value:	Units:
LCA	Global Warming Potential (GWP)	63.376654	kg CO_2-eq. / FU
	Ozone Depletion	0.000001	kg CFC-11-eq. / FU
	Mineral Resource Depletion	1.781505	kg Cu-eq. / FU
	Freshwater Eutrophication Potential	0.013813	kg P-eq. / FU
	Marine Eutrophication Potential	0.027154	kg N-eq. / FU
	Acidification Potential	0.137608	kg SO_2-eq. / FU
	Water Use	0.110454	m^3 / FU
TEA	Energy Demand	26,900	MJ / FU
	Energy Efficiency (%)	0.9	%
	Mass Efficiency (%)	0.982	%
	Est. Purchase Price (2022 £)	617.35	2022 £ / FU
SIA	Occupational Health and Safety (OSH)	0.611831817	-
	Child Labour	0.607493035	-
	Forced Labour	0.693382486	-
	Access to Electricity	0.476854934	-
	Access to Water	0.498116751	-
	Land Use Change	0.194659486	-
	Utilisation of Hazardous Materials	0.591436178	-

Spoke Data Sheet (I.D. 1.9)
(NH3 from Biogas fed Steam Methane Reformation & Haber Bosch)

Inventory Overview:

Quantity:	Character:
Input or Output?	Input
Reference Flow	1 tonne NH_3 via biogas fed Steam Methane Reformation & Haber Bosch
Scope	Cradle-to-Gate
Geographic Region	China
Timeframe	2022

System Boundary Block Flow Diagram (BFD):



Spoke Description:

This cradle-to-grave assessment of ammonia production assesses the coupled use of biomethane fed steam methane reforming and the Haber-Bosch process. It is assumed that all process heat (values obtained from literature) is provided through the combustion of biomethane. Steam methane reformation and Haber-Bosch models from the literature are identified for use (see table below). The impacts of raw material extraction and preparation for the process are examined using the appropriate Ecoinvent data sets reflecting the generation of biogas through the anaerobic digestion of biowaste and its subsequent treatment to produce biomethane. Beyond the biomethane feed, the SMR HB process model remains the same as the natural gas fed datasets. Biowaste is assumed to be procured sans burdens, and the biogenic carbon released through the combustion and reaction of biomethane is take as a zero burden in terms of impact indicators.

Spoke Sub-Section	Literature / Models Employed
Steam Methane Reformation	(D'Angelo, et al., 2021) (Boero, et al., 2021) (European Union Joint Research Council, 2007) (Van Herwijnen, et al., 1973)
Haber-Bosch Process	(Araújo & Skogestad, 2008) (Skogestad, 2004) (Morud & Skogestad, 1998)

In the first modelled step, hydrogen is produced from methane and, in the second, ammonia is synthesised via the Haber–Bosch reaction. Hydrogen is produced by primary and secondary steam methane reforming reactors (SMR) (Equation C-1). The first SMR reactor operates at around 850–900°C and 25–35 bar with the energy required for the endothermic reaction being provided by the combustion of methane. The second SMR reactor is autothermal, air is compressed and fed to the reactor to provide heat of reaction by partial oxidation of the reagents at 900–1000°C.

Equation 0-26

$$CH_4 + H_2O \leftrightarrow CO + 3H_2O$$

The SMR outlet mixture of carbon monoxide, hydrogen, and unreacted steam and methane are introduced into the two-stage water–gas shift (WGS) reactor to maximise CO conversion to hydrogen. The WGS reaction is exothermic, and heat must be removed to minimise CO concentration at equilibrium.

Equation 0-27

$$CO + H_2O \leftrightarrow CO_2 + H_2$$

The residual CO and CO2 in the H2-nitrogen mixture must be removed since they poison the HB catalyst.4 Hence, a methanation unit was placed after the MEA absorber to convert the residual CO and CO2 to methane and water. The vapour outlet of the absorption column is heated to 230 °C and fed to the methanation unit, which is modelled as a plug flow reactor implementing Equation C-3 & Equation C-4.

The residual methane present accumulates in the downstream synthesis loop (argon is also present but not modelled due to its presence in negligible mole fractions and removal in a purge stream).

Equation 0-28

$$CO + 3H_2 \leftrightarrow CH_4 + H_2O$$

Equation 0-29

$$CO_2 + 4H_2 \leftrightarrow CH_4 + 2H_2O$$

Although the steam methane reforming reactions are endothermic, the high reaction temperature and the need to cool substantially for the water gas shift reaction means that there is substantial waste heat available. This heat is used for raising high-pressure steam, which is expanded in steam turbines for compression, mainly used for compression of the feed in the Haber Bosch loop and the reformer combustion air compressor, which are the largest two energy users. The use of methane as feedstock inevitably leads to significant CO2 emissions from the process, and this is further compounded by the use of methane as fuel for the primary reformer furnace. The reaction kinetics are reported in Herwijnen et al. (1973), At the selected operating pressure, the conversion of CO2 and CO is 100%.

The H2 mixture is compressed to 196.3 bar, mixed with the recycle stream from the NH3 reactor, and then sent to a flash operating at the same pressure and 42 °C. The liquid outlet, rich in NH3, is sent to a flash unit, reaching an NH3 purity of ~98 mol% at the bottom.

The Haber-Bosch reaction system is modelled as a series of adiabatic plug-flow reactors with a void fraction of 33%, loaded with an iron-based catalyst. The kinetic model of the main reaction was directly adapted from the original reference (Morud & Skogestad, 1998) (Equation 0-5).

Equation 0-30

$$N_2 + 3H_2 \leftrightarrow 2NH_3$$

A nitrogen conversion of 25.3% is achieved inside the reactor. The reactor outlet is then cooled down to 27.1 °C and mixed with the fresh feed. It is then sent to the first flash, separating NH_3 from the remaining compounds and closing the loop.

Boundary Flows:

Classification:	Type:	Description:	Notation:
Input(s)	Raw material extraction	Ecoinvent used to evaluate the impact of feedstock extraction from the environment	N/A
Output(s)	Stream 10	CO_2 purge from WGS	10
	Stream 13	Water outlet from condenser	13
	Stream 19	Ammonia product (liquid)	19
	Stream 21	Haber Bosch loop purge stream	21
	Stream 26	Impacts and emissions associated with raw material extraction and preparation	26
	Stream 27	Impacts associated with the construction and operation of methane fired heating equipment	27

Process Units Included:

Classification:	Type:	Description:
Primary	SMR 1	First SMR, operating at 60% conversion
	SMR 2	Second SMR, achieving a 96.1% overall efficiency
	WGS Reactor	Conversion of CO to CO_2 through the
	Separation Column	Removes CO_2 from the WGS product stream
	Methanation Reactor	Converts remaining traces of CO and CO_2 back to CH_4 to prevent catalyst poisoning within the downstream HB reactor
	HB Reactor	Production of ammonia with a recycle loop to improve efficiency.
Secondary	HX 1	-
	Compressor 1	-
	HX2	-
	Condenser	-
	Compressor 2	-
	Mixer 1	-
	Mixer 2	-
	Flash Drum	-
	Splitter 1	-
	Compressor 3	-
	HX 3	-

Assumptions:

Aspect:	Assumption(s):

System Boundary	• Ecoinvent datasets assumed to be reflective of the secondary feedstock production (ReCiPe Midpoint (H) characterisation)
	• Electricity generation is handled on-site via a steam turbine fed by process steam from biomethane combustion
	• Heat is supplied via biomethane combustion
	  ○ Mol/m3 supplied is evaluated using ideal gas law (5 Bar, 298.15 K)
	  ○ 4.5 GJ / tonne NH_3 heat requirement (German UBA, 2000) [384]
	• CO_2 removal within SMR is achieved using Selexol due to its widespread adoption (European Union Joint Research Council, 2007)
	• Biomethane production from biowaste via anaerobic digestion and pressure swing absorption is as modelled as the CH_4 feedstock.
	• Excludes SMR/HB plant construction & decommissioning
	• Costing data taken from literature for green ammonia (natural gas fed without CCS) in Asia (S&P Global Commodity Insights, 2023)

Mass balance	• 60% conversion efficiency within primary SMR (European Union Joint Research Council, 2007) • 96.1% conversion efficiency within second SMR (derived from mass balance and primary data for outlet stream composition) (European Union Joint Research Council, 2007) • Steam to methane ratio of 3:1 (European Union Joint Research Council, 2007) • 98% conversion within WGS reactor (European Union Joint Research Council, 2007) • 100% CO & CO_2 conversion efficiency within the methanation reactor (D'Angelo, et al., 2021) • Methane combustion for steam generation assumes an optimal 90% combustion efficiency (Mickey, 2017) and 84.3% heat recovery (Najmi & Arhosazni, 2006)
Energy balance	• Average values for BAT plants (29.6 GJ/tonne NH_3) taken from an LCA/TEA with matching system boundaries [384]. This was then sense checked against a consideration of minimum energy required through enthalpy calculations. Energy supplied by menthane in SMR reactions is subsequently excluded as impacts are captured by the process' mass balance. • Methane energy content of 52 MJ/kg and sourcing from biowaste • Energy efficiency of methane burners assumed to be 90% as detailed in literature (Mickey, 2017)
Waste handling	• Gaseous emissions are directly vented.

	• Liquid effluents released to waterways.
Transportation	• Not included
Miscellaneous	• None

Stream Table:

Stream	Species In (kmol/hr)							Species In (kg/hr)							Totals
	CH4	H2O	CO	H2	CO2	N2	NH3	CH4	H2O	CO	H2	CO2	N2	NH3	
1	23.09642168	0	0	0	0	0	0	369.542747	0	0	0	0	0	0	*369.542747*
2	0	69.289265	0	0	0	0	0	0	1247.206771	0	0	0	0	0	*1247.206771*
3	9.238568672	55.431412	13.85785301	41.573559	0	0	0	147.817099	997.7654166	388.019884	83.147118	0	0	0	*1616.749518*
4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	*0.000000*
5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	*0.000000*
6	0.360304178	46.5531475	22.7361175	68.2083525	0	0	0	5.76486685	837.9566557	636.61129	136.416705	0	0	0	*1616.749518*
7	0.360304178	46.5531475	22.7361175	68.2083525	0	0	0	5.76486685	837.9566557	636.61129	136.416705	0	0	0	*1616.749518*
8	0.360304178	24.2717524	0.45472235	90.4897477	22.28139515	0	0	5.76486685	436.891543	12.7322258	180.979495	980.381387	0	0	*1616.749518*
9	0.360304178	24.2717524	0.45472235	90.4897477	22.28139515	0	0	5.76486685	436.891543	12.7322258	180.979495	980.381387	0	0	*1616.749518*
10	0	0	0	0	22.28139515	0	0	0	0	0	0	980.381387	0	0	*980.381387*
11	0.360304178	24.2717524	0.45472235	90.4897477	0	0	0	5.76486685	436.891543	12.7322258	180.979495	0	0	0	*636.368131*
12	0.815026528	24.7264747	0	89.1255806	0	0	0	13.0404245	445.0765453	0	178.251161	0	0	0	*636.368131*
13	0	24.7264747	0	0	0	0	0	0	445.0765453	0	0	0	0	0	*445.076545*
14	0.815026528	0	0	89.1255806	0	0	0	13.0404245	0	0	178.251161	0	0	0	*191.291586*
15	0.815026528	0	0	89.1255806	0	0	0	13.0404245	0	0	178.251161	0	0	0	*191.291586*
16	0	0	0	0	0	29.7364711	0	0	0	0	0	0	832.621191	0	*832.621191*
17	0.815026528	0	0	89.1255806	0	29.7364711	0	13.0404245	0	0	178.251161	0	832.621191	0	*1023.912777*
18	20.34251538	0	0	369.536571	0	108.493132	139.26747	325.480246	0	0	739.073141	0	3037.8077	2367.546998	*6469.908089*
19	0	0	0	0.8412385	0	0.3094244	58.8235294	0	0	0	1.682477	0	8.6638833	1000	*1010.346360*
20	20.34251538	0	0	368.695332	0	108.183708	80.4439411	325.480246	0	0	737.390664	0	3029.14382	1367.546998	*5459.561729*
21	0.815026528	0	0	0.03784118	0	0.0114979	0.00771378	13.0404245	0	0	0.07568236	0	0.3219411	0.131134237	*13.569182*
22	19.52748885	0	0	368.657491	0	108.17221	80.4362273	312.439822	0	0	737.314982	0	3028.82188	1367.415864	*5445.992546*
23	19.52748885	0	0	368.657491	0	108.17221	80.4362273	312.439822	0	0	737.314982	0	3028.82188	1367.415864	*5445.992546*
24	19.52748885	0	0	368.657491	0	108.17221	80.4362273	312.439822	0	0	737.314982	0	3028.82188	1367.415864	*5445.992546*
25	19.52748885	0	0	280.41099	0	78.7566611	139.26747	312.439822	0	0	560.82198	0	2205.18651	2367.546998	*5445.995312*
26	Boundary flow with impacts assessed through Ecoinvent data sets: ‘treatment of biowaste by anaerobic digestion - RoW – biogas’ & biogas purification to biomethane by pressure swing adsorption - RoW - biomethane, high pressure’														N/A
27	Boundary flow with impacts assessed through Ecoinvent data set: treatment of biowaste by anaerobic digestion - RoW – biogas’ & biogas purification to biomethane by pressure swing adsorption - RoW - biomethane, high pressure’ & stochiometric evaluation of emissions (CH4 & CO2) excluding biogenic carbon														N/A

Lifecycle Assessment (LCA) Data:

Indicator	Value	Unit
Global Warming Potential (GWP)	63.376654	kg CO_2-eq. / FU
Ozone Depletion	0.000001	kg CFC-11-eq. / FU
Mineral Resource Depletion	1.781505	kg Cu-eq. / FU
Freshwater Eutrophication Potential	0.013813	kg P-eq. / FU
Marine Eutrophication Potential	0.027154	kg N-eq. / FU
Acidification Potential	0.137608	kg SO_2-eq. / FU
Water Use	0.110454	m^3 / FU

Technoeconomic Assessment (TEA) Data:

Variable	Value	Unit
Energy Requirement	26,900	MJ / FU
Total:	26,900	MJ / FU

Variable	Value	Unit
Energy Input	5,000	MJ / FU
Theoretical Energy Requirement	4,500	MJ / FU
Achieved Energy Efficiency	0.9	Decimal
Overall Relative Mass Efficiency:	0.9	Decimal

Variable	Value	Unit
Mass Fed (Total)	2449.37	kg / FU
Mass of Product	1000	kg / FU
Theoretical Maximum Mass Efficiency	0.4157	Decimal
Achieved Mass Efficiency	0.4083	Decimal
Overall Relative Mass Efficiency:	0.982	Decimal

Flow	Price Data	Data Currency	Year	Price 2022£ / FU:	Quantity Req.:	Total Value:	Unit
1 Tonne	781.45	USD	2023 (Oct)	617.35	1	617.35	£ / FU
					Total:	617.35	£ / FU

Social Impact Assessment (SIA) Data:

Indicator	Sub-Indicator(s)	Sub-Indicator Value(s)	Final Aggregated Indicator Score
Occupational Health and Safety (OSH)	Accidents causing >4 days' absence	0.586213385	0.694329585
	Work-related disease	0.754901847	
	Work-related mortality	0.714012633	
Child Labour	Non-hazardous	0.740585774	0.617058249
	Hazardous		
	Vulnerability	0.493530724	
Forced Labour	Prevalence	0.973555901	0.733543312119765
	Vulnerability	0.493530724	
Access to Electricity	Energy imports, net (% of energy use)	0.849781993	0.491839919
	Fossil fuel energy consumption (% of total)	0.123295692	
	Electric power consumption (kWh per capita)	0.070600891	
	Renewable energy consumption (% of total final energy consumption)	0.1445	
Access to Water	Freshwater withdrawal as % of total	0.791635859	0.679709488
	Water Stress	0.567783117	
Land Use Change	-	0.277838446	0.277838445646095
Utilisation of Hazardous Materials	Deaths caused by dangerous substances per 10,000 workers	0.754900315	0.754900315

Aggregated Final Objective Indicator Scores:

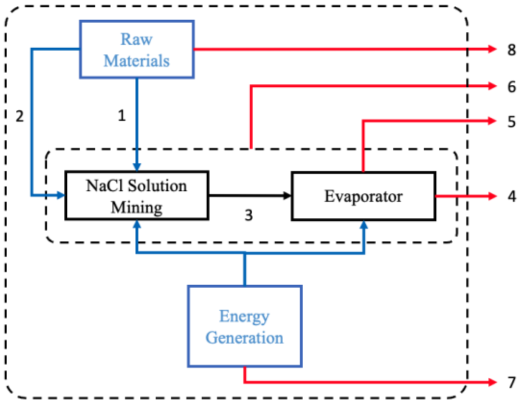
Assessment Strand:	Indicator:	Value:	Units:
LCA	Global Warming Potential (GWP)	63.376654	kg CO_2-eq. / FU
	Ozone Depletion	0.000001	kg CFC-11-eq. / FU
	Mineral Resource Depletion	1.781505	kg Cu-eq. / FU
	Freshwater Eutrophication Potential	0.013813	kg P-eq. / FU
	Marine Eutrophication Potential	0.027154	kg N-eq. / FU
	Acidification Potential	0.137608	kg SO_2-eq. / FU
	Water Use	0.110454	m^3 / FU
TEA	Energy Demand	26,900	MJ / FU
	Energy Efficiency (%)	0.9	%
	Mass Efficiency (%)	0.982	%
	Est. Purchase Price (2022 £)	617.35	2022 £ / FU
SIA	Occupational Health and Safety (OSH)	0.694329585	-
	Child Labour	0.617058249	-
	Forced Labour	0.733543312	-
	Access to Electricity	0.491839919	-
	Access to Water	0.679709488	-
	Land Use Change	0.277838446	-
	Utilisation of Hazardous Materials	0.754900315	-

Spoke Data Sheet (I.D. 2.1)
(NaCl from Solution Mining with Natural Gas Heat Provision)

Inventory Overview:

Quantity:	Character:
Input or Output?	Input
Reference Flow	1 tonne NaCl via solution mining
Scope	Cradle-to-Gate
Geographic Region	India
Timeframe	2022

System Boundary Block Flow Diagram (BFD):



Spoke Description:

Underground salt deposits can be utilised through solution mining. In the extraction process, a well is bored into the deposit of soluble salts, followed by water injection. The salt, in this case NaCl, dissolves into the injected water and is recovered to the surface. Once at the surface, the NaCl brine is pumped to evaporating units to increase concentration to the desired level. For the production of soda ash via the Hou process, an NaCl concentration of 25.6 wt% is desired. The provision of energy for the evaporation phase is handled through the combustion of natural gas. Electrical energy is representative of regional grid mixes.

Ecoinvent V3.8 datasets are available for the solution mining process itself, inclusive of drilling, pumping and infrastructure. Beyond this the evaporation of excess water must be considered. For this, additional Ecoinvent V3.8 datasets are incorporated, detailed in the table below.

Production Step	Dataset / Model Used
Solution mining	Ecoinvent: ‘sodium chloride production, brine solution - RoW - sodium chloride, brine solution’
Water Feed	Ecoinvent: ‘tap water production, underground water with chemical treatment - RoW - tap water’
Heat Generation (Evaporation)	Ecoinvent: 'heat production, natural gas, at industrial furnace >100kW - RoW - heat, district or industrial, natural gas'

Boundary Flows:

Classification:	Type:	Description:	Notation:
Input(s)	Raw material extraction	Ecoinvent used to evaluate the impact of feedstock extraction from the environment (water and salt)	N/A
Output(s)	Stream 4	NaCl product	4
	Stream 5	Water vapour from evaporation	5
	Stream 6	Emissions associated with solution mining of raw NaCl	6
	Stream 7	Emissions associated with energy generation	7

Process Units Included:

Classification:	Type:	Description:
Primary	Solution mining loop	Includes the pumping of water into and recovery of brine from the solution mining
	Evaporator	The concentration of NaCl to wt% required by the Hou process.

Assumptions:

Aspect:	Assumption(s):
System Boundary	• Ecoinvent datasets are assumed to be reflective of the secondary feedstock production (ReCiPe Midpoint (H) characterisation). • Economic data is retrieved for the market average price of brine in 2022 (U.S. Department of the Interior, 2023) • Economic data for industrial natural gas prices per MJ of natural gas in India is obtained from an Indian Government Report (Ministry of Petroleum and natural Gas, 2022).
Mass balance	• Final NaCl brine should achieve 25.6 wt% (Kasikowski, et al., 2004) for use in the Hou process • NaCl deposit is assumed to be pure with no requirement for further purification. • The mass efficiency of the system is based on the salt extracted from deposits. As no salt is lost in the concentrating step, the efficiency is therefore 100%
Energy balance	• The heat capacity of 20% brine (25% not available) identified in the literature (3341.4 J/kg.K) and assumed to be constant over the 25-100ºC temperature range (Ramalingam & Arumugam, 2012). • The latent heat of water identified in the literature as 2260 kJ/kg / 40.8 kJ/mol (Datt, 2011). • Boiling point of 20 wt% brine identified as 108.7ºC (Hocking, 2005) • Energy efficiency of heat provision is assumed to be equal to that of typical industrial furnace and heat exchanger arrangements (90%) (Mickey, 2017).
Waste handling	• Gaseous emissions are directly vented. • Liquid effluents released to waterways
Transportation	• Not included
Miscellaneous	• None

Stream Table:

Stream	Species (kmol/hr)		Species In (kg/hr)		Total
	H2O	NaCl	H2O	NaCl	
1	354.432466	0.0000000	6385.101	0.000	6385.101
2	0	17.11156742	0.000	1000.000	1000.000
3	354.432466	17.1115674	6385.101	1000.000	7385.101
4	161.3238968	17.1115674	2906.250	1000.000	3906.250
5	193.1085693	0.0000000	3478.851	0.000	3478.851
6	Boundary flow with impacts assessed through Ecoinvent data set: 'sodium chloride production, brine solution - RoW - sodium chloride, brine solution'				N/A
7	Boundary flow with impacts assessed through Ecoinvent data set: 'heat production, natural gas, at industrial furnace >100kW - RoW - heat, district or industrial, natural gas'				

Lifecycle Assessment (LCA) Data:

Indicator	Value	Unit
Global Warming Potential (GWP)	1746.403628	kg CO_2-eq. / FU
Ozone Depletion	0.000101	kg CFC-11-eq. / FU
Mineral Resource Depletion	383.477856	kg Cu-eq. / FU
Freshwater Eutrophication Potential	1.138309	kg P-eq. / FU
Marine Eutrophication Potential	1.303161	kg N-eq. / FU
Acidification Potential	7.040655	kg SO_2-eq. / FU
Water Use	11.102931	m^3 / FU

Technoeconomic Assessment (TEA) Data:

Variable	Value	Unit
Solution Mining	2496.164	MJ / FU
Evaporator	11025.689	MJ / FU
Total:	13521.853	MJ / FU

Variable	Value	Unit
Energy Input	13521.853	MJ / FU
Theoretical Energy Requirement	12419.284	MJ / FU
Achieved Energy Efficiency	0.91846	Decimal
Overall Relative Energy Efficiency:	0.91846	Decimal

Variable	Value	Unit
Mass Fed (Total)	7385.101	kg / FU
Mass of Product	1000	kg / FU
Theoretical Maximum Mass Efficiency	1	Decimal
Achieved Mass Efficiency	1	Decimal
Overall Relative Mass Efficiency:	1	Decimal

Flow	Price Data / FU	Data Currency	Year	Price 2022£ / FU:	Quantity Req. (FU):	Total Value:	Unit
Raw Brine	8.5	USD	2022	6.898	1	6.898	£ / FU
Natural Gas	0.00578	USD	2022	0.00469	13521.853	63.41749057	£ / FU
					Total:	70.31549057	£ / FU

Social Impact Assessment (SIA) Data:

Indicator	Sub-Indicator(s)	Sub-Indicator Value(s)	Final Aggregated Indicator Score
Occupational Health and Safety (OSH)	Accidents causing >4 days' absence	0.586213385	0.694329585
	Work-related disease	0.754901847	
	Work-related mortality	0.714012633	
Child Labour	Non-hazardous	0.740585774	0.617058249
	Hazardous		
	Vulnerability	0.493530724	
Forced Labour	Prevalence	0.973555901	0.733543312119765
	Vulnerability	0.493530724	
Access to Electricity	Energy imports, net (% of energy use)	0.849781993	0.491839919
	Fossil fuel energy consumption (% of total)	0.123295692	
	Electric power consumption (kWh per capita)	0.070600891	
	Renewable energy consumption (% of total final energy consumption)	0.1445	
Access to Water	Freshwater withdrawal as % of total	0.791635859	0.679709488
	Water Stress	0.567783117	
Land Use Change	-	0.277838446	0.277838445646095
Utilisation of Hazardous Materials	Deaths caused by dangerous substances per 10,000 workers	0.754900315	0.754900315

Aggregated Final Objective Indicator Scores:

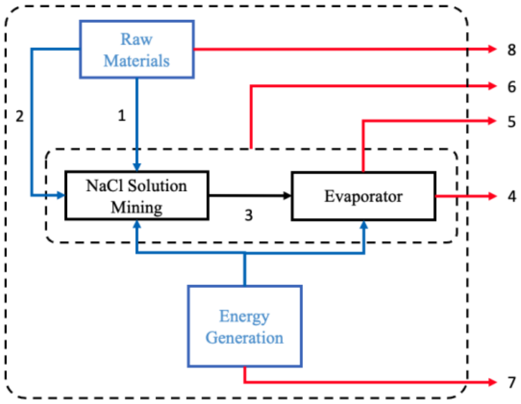
Assessment Strand:	Indicator:	Value:	Units:
LCA	Global Warming Potential (GWP)	1593.688118	kg CO_2-eq. / FU
	Ozone Depletion	0.000058	kg CFC-11-eq. / FU
	Metal Resource Depletion	140.832203	kg Cu-eq. / FU
	Freshwater Eutrophication Potential	0.434176	kg P-eq. / FU
	Marine Eutrophication Potential	1.168815	kg N-eq. / FU
	Acidification Potential	7.115654	kg SO_2-eq. / FU
	Water Use	3.028813	m^3 / FU
TEA	Energy Demand	13521.853	MJ / FU
	Energy Efficiency (%)	0.91846	%
	Mass Efficiency (%)	1	%
	Est. Purchase Price (2022 £)	70.31549057	2022 £ / FU
SIA	Occupational Health and Safety (OSH)	0.611831817	-
	Child Labour	0.607493035	-
	Forced Labour	0.693382486	-
	Access to Electricity	0.476854934	-
	Access to Water	0.498116751	-
	Land Use Change	0.194659486	-
	Utilisation of Hazardous Materials	0.591436178	-

Spoke Data Sheet (I.D. 2.2)
(NaCl from Direct Solution Mining with Natural Gas Heat Provision)

Inventory Overview:

Quantity:	Character:
Input or Output?	Input
Reference Flow	1 tonne NaCl via solution mining
Scope	Cradle-to-Gate
Geographic Region	China
Timeframe	2022

System Boundary Block Flow Diagram (BFD):



Spoke Description:

Underground salt deposits can be utilised through solution mining. In the extraction process, a well is bored into the deposit of soluble salts, followed by water injection. The salt, in this case NaCl, dissolves into the injected water and is recovered to the surface. Once at the surface, the NaCl brine is pumped to evaporating units to increase concentration to the desired level. For the production of soda ash via the Hou process, an NaCl concentration of 25.6 wt% is desired. The provision of energy for the evaporation phase is handled through the combustion of natural gas. Electrical energy is representative of regional grid mixes.

Ecoinvent V3.8 datasets are available for the solution mining process itself, inclusive of drilling, pumping and infrastructure. Beyond this the evaporation of excess water must be considered. For this, additional Ecoinvent V3.8 datasets are incorporated, detailed in the table below.

Production Step	Dataset / Model Used
Solution mining	Ecoinvent: 'sodium chloride production, brine solution - RoW - sodium chloride, brine solution'
Water Feed	Ecoinvent: 'tap water production, underground water with chemical treatment - RoW - tap water'
Heat Generation (Evaporation)	Ecoinvent: 'heat production, natural gas, at industrial furnace >100kW - RoW - heat, district or industrial, natural gas'

Boundary Flows:

Classification:	Type:	Description:	Notation:
Input(s)	Raw material extraction	Ecoinvent used to evaluate the impact of feedstock extraction from the environment (water and salt)	N/A
Output(s)	Stream 4	NaCl product	4
	Stream 5	Water vapour from evaporation	5
	Stream 6	Emissions associated with solution mining of raw NaCl	6
	Stream 7	Emissions associated with energy generation	7

Process Units Included:

Classification:	Type:	Description:
Primary	Solution mining loop	Includes the pumping of water into and recovery of brine from the solution mining
	Evaporator	The concentration of NaCl to wt% required by the Hou process.

Assumptions:

Aspect:	Assumption(s):
System Boundary	• Ecoinvent datasets are assumed to be reflective of the secondary feedstock production (ReCiPe Midpoint (H) characterisation). • Economic data is retrieved for the market average price of brine in 2022 (U.S. Department of the Interior, 2023) • Economic data for industrial natural gas prices per MJ of natural gas in China is obtained from an IEA Report (International Energy Agency, 2023).
Mass balance	• Final NaCl brine should achieve 25.6 wt% (Kasikowski, et al., 2004) for use in the Hou process • NaCl deposit is assumed to be pure with no requirement for further purification. • The mass efficiency of the system is based on the salt extracted from deposits. As no salt is lost in the concentrating step, the efficiency is therefore 100%
Energy balance	• The heat capacity of 20% brine (25% not available) identified in the literature (3341.4 J/kg.K) and assumed to be constant over the 25-100ºC temperature range (Ramalingam & Arumugam, 2012). • The latent heat of water identified in the literature as 2260 kJ/kg / 40.8 kJ/mol (Datt, 2011). • Boiling point of 20 wt% brine identified as 108.7ºC (Hocking, 2005) • Energy efficiency of heat provision is assumed to be equal to that of typical industrial furnace and heat exchanger arrangements (90%) (Mickey, 2017).
Waste handling	• Gaseous emissions are directly vented. • Liquid effluents released to waterways
Transportation	• Not included
Miscellaneous	• None

Stream Table:

Stream	Species (kmol/hr)		Species In (kg/hr)		Total
	H2O	NaCl	H2O	NaCl	
1	354.432466	0.0000000	6385.101	0.000	6385.101
2	0	17.11156742	0.000	1000.000	1000.000
3	354.432466	17.1115674	6385.101	1000.000	7385.101
4	161.3238968	17.1115674	2906.250	1000.000	3906.250
5	193.1085693	0.0000000	3478.851	0.000	3478.851
6	Boundary flow with impacts assessed through Ecoinvent data set: 'sodium chloride production, brine solution - RoW - sodium chloride, brine solution'				N/A
7	Boundary flow with impacts assessed through Ecoinvent data set: 'heat production, natural gas, at industrial furnace >100kW - RoW - heat, district or industrial, natural gas'				

Lifecycle Assessment (LCA) Data:

Indicator	Value	Unit
Global Warming Potential (GWP)	1746.403628	kg CO_2-eq. / FU
Ozone Depletion	0.000101	kg CFC-11-eq. / FU
Mineral Resource Depletion	383.477856	kg Cu-eq. / FU
Freshwater Eutrophication Potential	1.138309	kg P-eq. / FU
Marine Eutrophication Potential	1.303161	kg N-eq. / FU
Acidification Potential	7.040655	kg SO_2-eq. / FU
Water Use	11.102931	m^3 / FU

Technoeconomic Assessment (TEA) Data:

Variable	Value	Unit
Solution Mining	2496.164	MJ / FU
Evaporator	11025.689	MJ / FU
Total:	13521.853	MJ / FU

Variable	Value	Unit
Energy Input	13521.853	MJ / FU
Theoretical Energy Requirement	12419.284	MJ / FU
Achieved Energy Efficiency	0.91846	Decimal
Overall Relative Energy Efficiency:	0.91846	Decimal

Variable	Value	Unit
Mass Fed (Total)	7385.101	kg / FU
Mass of Product	1000	kg / FU
Theoretical Maximum Mass Efficiency	1	Decimal
Achieved Mass Efficiency	1	Decimal
Overall Relative Mass Efficiency:	1	Decimal

Flow	Price Data / FU	Data Currency	Year	Price 2022£ / FU:	Quantity Req. (FU):	Total Value:	Unit
Raw Brine	8.5	USD	2022	6.898	1	6.898	£ / FU
Natural Gas	0.018	USD	2022	0.0146	13521.853	197.52	£ / FU
					Total:	204.418	£ / FU

Social Impact Assessment (SIA) Data:

Indicator	Sub-Indicator(s)	Sub-Indicator Value(s)	Final Aggregated Indicator Score
Occupational Health and Safety (OSH)	Accidents causing >4 days' absence	0.586213385	0.694329585
	Work-related disease	0.754901847	
	Work-related mortality	0.714012633	
Child Labour	Non-hazardous	0.740585774	0.617058249
	Hazardous		
	Vulnerability	0.493530724	
Forced Labour	Prevalence	0.973555901	0.733543312119765
	Vulnerability	0.493530724	
Access to Electricity	Energy imports, net (% of energy use)	0.849781993	0.491839919
	Fossil fuel energy consumption (% of total)	0.123295692	
	Electric power consumption (kWh per capita)	0.070600891	
	Renewable energy consumption (% of total final energy consumption)	0.1445	
Access to Water	Freshwater withdrawal as % of total	0.791635859	0.679709488
	Water Stress	0.567783117	
Land Use Change	-	0.277838446	0.277838445646095
Utilisation of Hazardous Materials	Deaths caused by dangerous substances per 10,000 workers	0.754900315	0.754900315

Aggregated Final Objective Indicator Scores:

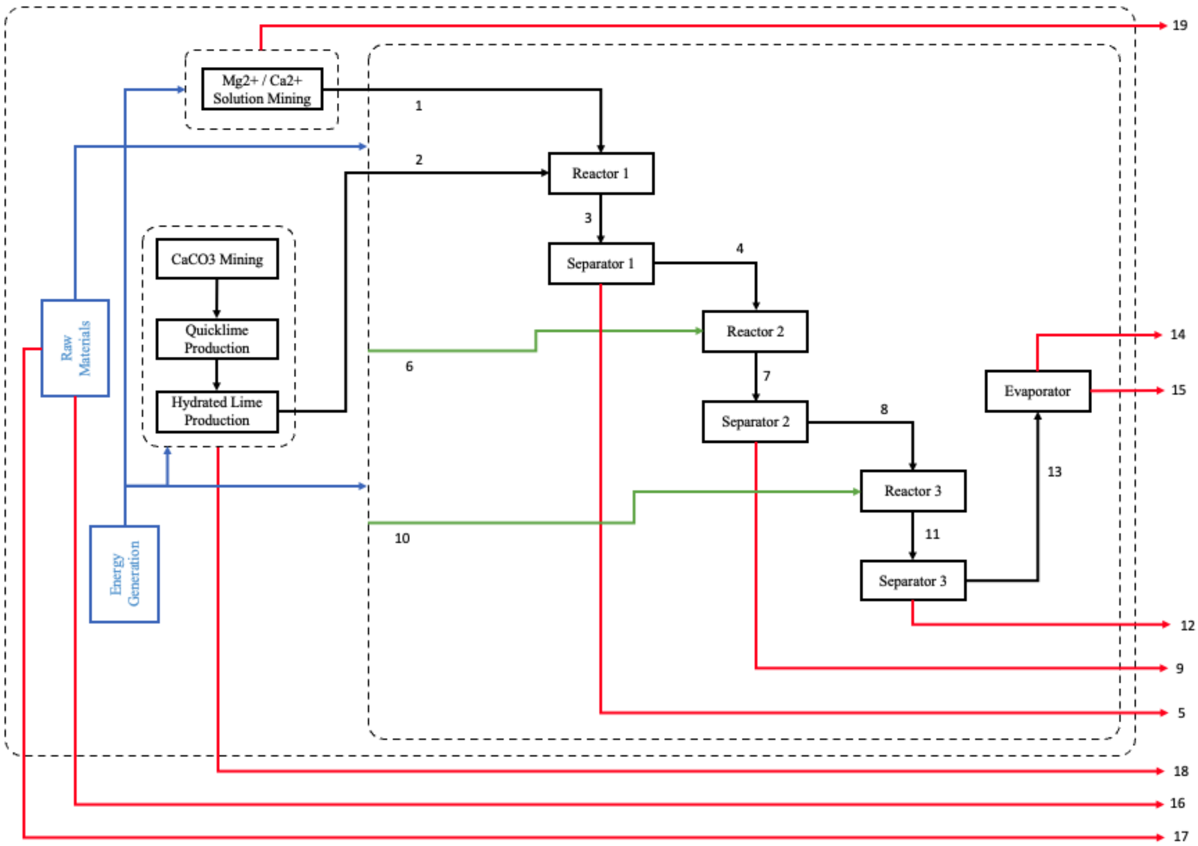
Assessment Strand:	Indicator:	Value:	Units:
LCA	Global Warming Potential (GWP)	1593.688118	kg CO_2-eq. / FU
	Ozone Depletion	0.000058	kg CFC-11-eq. / FU
	Metal Resource Depletion	140.832203	kg Cu-eq. / FU
	Freshwater Eutrophication Potential	0.434176	kg P-eq. / FU
	Marine Eutrophication Potential	1.168815	kg N-eq. / FU
	Acidification Potential	7.115654	kg SO_2-eq. / FU
	Water Use	3.028813	m^3 / FU
TEA	Energy Demand	13521.853	MJ / FU
	Energy Efficiency (%)	0.91846	%
	Mass Efficiency (%)	1	%
	Est. Purchase Price (2022 £)	204.418	2022 £ / FU
SIA	Occupational Health and Safety (OSH)	0.694329585	-
	Child Labour	0.617058249	-
	Forced Labour	0.733543312	-
	Access to Electricity	0.491839919	-
	Access to Water	0.679709488	-
	Land Use Change	0.277838446	-
	Utilisation of Hazardous Materials	0.754900315	-

Spoke Data Sheet (I.D. 2.3)
(NaCl from Solution Mining of Mg^{2+} & Ca^{2+} Brine with Ion Exchange and Purification)

Inventory Overview:

Quantity:	Character:
Input or Output?	Input
Reference Flow	1 tonne NaCl via solution mining of Mg^{2+} & Ca^{2+} Brines
Scope	Cradle-to-Gate
Geographic Region	India
Timeframe	2022

System Boundary Block Flow Diagram (BFD):



Spoke Description:

Calcium and magnesium-rich brine is obtained from natural deposits using electrically powered pumping equipment and freshwater. Ecoinvent data is used to quantify the impacts associated with the solution mining (see dataset details in the table below). This solution mining LCI data only covers the extraction process, and it's associated energy, operational, and infrastructure emissions.

Once extracted, the raw brine must be treated to generate NaCl. In this process the brine is treated with $Ca(OH)_2$, Na_2SO_4, and Na_2CO_3 to remove Mg^{2+} ions, Ca^{2+} ions, and the residual Ca^{2+} ions, respectively (see reaction equations below). Using this route, a large proportion of Ca^{2+} ions are deposited in the form of $CaSO_4$ instead of $CaCO_3$, which reduces the soda ash consumption; in addition, $CaSO_4$ and $CaCO_3$ can accelerate further precipitation of $Mg(OH)_2$. After each purification step filters are used to remove solid precipitates.

Equation 0-31

$$MgCl_2 + Ca(OH)_2 \rightarrow Mg(OH)_2 + CaCl_2$$

Equation 0-32

$$Na_2SO_4 + CaCl_2 \rightarrow CaSO_4 + 2NaCl$$

Equation 0-33

$$Na_2CO_3 + CaCl_2 \rightarrow 2NaCl + CaCO_3$$

Na_2SO_4 is obtained through the mining of natural deposits (anhydrous). $Ca(OH)_2$ is obtained through the mining of limestone, it's calcination to form anhydrous quicklime pieces, followed by slaking to produce hydrated lime. Due to the sequential steps in this process, multiple Ecoinvent V3.8 datasets have been aggregated to quantify cradle-to-gate impacts (see details of utilised datasets in the table below). Electricity requirements for the solution mining stage and mining of Na_2SO_4 are reflective of the average European grid mix (a limitation of the Ecoinvent datasets). Heat supplied is based on an Ecoinvent v3.8 data set non-natural gas source, including a mix of; burning biomethane in gas turbine; biogas in co-gen gas engine; anthracite, coal, lignite briquettes and coke in stove; hardwood, logs, softwood, wood chips, wood pellets in furnaces and wood heaters; light fuel oil in boilers. Also contributing are heat from heat pumps and solar collectors. The dataset is targeted for district and industrial-scale heating such as that observed in this system. Additional electricity requirements are evaluated based on the grid mix of the country examined.

After obtaining the NaCl brine, excess water must be evaporated to deliver the required concentration for use in the production of soda ash via the Hou process (25.6 wt%). The heat required for this process is assumed to be delivered through the combustion of natural gas.

Production Step	Dataset / Model Used
Solution mining	Ecoinvent: sodium chloride production, brine solution - RoW - sodium chloride, brine solution
Brine Purification	Brine purification via Na2SO4 and Na2CO3 addition [398] Ecoinvent Supporting Data: 'Soda production, Solvay process - RoW - soda ash, light, crystalline, heptahydrate', & 'sodium sulfate production, from natural sources - RoW - sodium sulfate, anhydrite'
Hydrated Lime Production	Ecoinvent Datasets: 'lime production, hydrated, loose weight - RoW - lime, hydrated, loose weight' & 'quicklime production, in pieces, loose - RoW - quicklime, in pieces, loose' & 'limestone quarry operation - RoW - limestone, unprocessed'
Process Heat	Ecoinvent Dataset: 'market for heat, district or industrial, other than natural gas - RoW - heat, district or industrial, other than natural gas'

Boundary Flows:

Classification:	Type:	Description:	Notation:
Input(s)	Raw material extraction	Ecoinvent used to evaluate the impact of feedstock extraction from the environment	N/A
Output(s)	Stream 5	Precipitated $Mg(OH)_2$ from separator 1	5
	Stream 9	Precipitated $CaSO_4$ from separator 2	9
	Stream 12	Precipitated $CaCO_3$ with trace contaminants from separator 3	12
	Stream 14	Water vapour emission from the concentration of brine in the evaporator	14
	Stream15	NaCl brine product	15
	Stream 16	Emissions associated with Na_2SO_4 feedstock production	16
	Stream 17	Emissions associated with Na_2CO_3 feedstock production	17
	Stream 18	Emissions associated with $Ca(OH)_2$ feedstock production	18
	Stream 19	Emissions associated with raw brine (Mg^{2+}/Ca^{2+}) solution mining	19

Process Units Included:

Classification:	Type:	Description:
Primary	Reactor 1	Reaction precipitates magnesium ions in the form of $Mg(OH)_2$ through the addition of $Ca(OH)_2$ to raw brine.
	Reactor 2	Addition of Na_2SO_4 to the remaining raw brine results in the precipitation of calcium ions in the from of $CaSO_4$.
	Reactor 3	Addition of soda ash to brine solution removes any remaining calcium ions in the form of $CaCO_3$.
	Evaporator	The concentration of NaCl to wt% required by the Hou process
Secondary	Separator 1	Removal of the precipitated products of brine purification.
	Separator 2	
	Separator 3	

Assumptions:

Aspect:	Assumption(s):
System Boundary	• Ecoinvent datasets assumed to be reflective of the secondary feedstock production (ReCiPe Midpoint (H) characterisation). A secondary sub-system is defined for the production of hydrated lime ($Ca(OH)_2$) due to the absence of cradle-to-gate LCI data within Ecoinvent. • The Ecoinvent sodium chloride solution mining dataset is used as a proxy for the impacts of calcium and magnesium solution mining. The employed technologies and operating conditions are highly comparable (Paidoussis, 2014). • Raw brine prices are not presented by [398]. Therefore, economic data is retrieved for the market average price of brine in 2022 (U.S. Department of the Interior, 2023) • Economic data for industrial natural gas prices per MJ of natural gas in India is obtained from an Indian Government Report (Ministry of Petroleum and natural Gas, 2022). • 2022 USD to GBP conversion rate is given as 0.7501 as the year's average (Exchange Rates UK, 2024)
Mass balance	• Raw brine ion composition is derived from Cao, et al. [398] • Final NaCl brine should achieve 25.6 wt% (Kasikowski, et al., 2004) for use in the Hou process • First purification step exhibits a 90.05% efficiency with respect to magnesium ion utilisation [398]. • Second and third purification step efficiencies assumed to be 100% due to irreversibility, and previous work by Cao, et al. [398]. • Mass efficiency of the system is based on the purification loop and thus utilisation of the Ca^{2+} and Mg^{2+}. This is also reflective of the fact that supply chain data get opaquer as the distance to the overall assessment's 'hub' increases.
Energy balance	• The energy demand of the purification steps involves only the pumping and agitation of liquid and conveying of solids. • Covers the energy demand associated with the extraction and handling of raw materials prior to the purification step. • Energy efficiency of heat provision is assumed to be equal to that of typical industrial furnace and heat exchanger arrangements (90%) (Mickey, 2017).
Waste handling	• Gaseous emissions are directly vented. • Liquid effluents released to waterways
Transportation	• Not included
Miscellaneous	• None

Stream Table:

Stream	Species (kmol/hr)													Species In (kg/hr)													Total
	H2O	CaCl2	Ca(OH)2	CaSO4	CaCO3	MgCl2	Mg(OH)2	MgSO4	4MgCO3.Mg(OH)2.4H2O	NaCl	Na2SO4	Na2CO3	CO2	H2O	CaCl2	Ca(OH)2	CaSO4	CaCO3	MgCl2	Mg(OH)2	MgSO4	4MgCO3.Mg(OH)2.4H2O	NaCl	Na2SO4	Na2CO3	CO2	
1	443.900	1.977	0.000	0.000	0.000	7.410	0.000	0.000	0.000	0.030	0.000	0.000	0.000	7996.856	219.391	0.000	0.000	0.000	705.467	0.000	0.000	0.000	1.767	0.000	0.000	0.000	8923.481
2	35.478	0.000	6.706	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	639.137	0.000	496.819	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1135.956
3	479.378	8.682	0.000	0.000	0.000	0.704	6.706	0.000	0.000	0.030	0.000	0.000	0.000	8635.993	963.579	0.000	0.000	0.000	67.019	391.069	0.000	0.000	1.767	0.000	0.000	0.000	10059.428
4	474.596	8.682	0.000	0.000	0.000	0.704	0.000	0.000	0.000	0.030	0.000	0.000	0.000	8549.847	963.579	0.000	0.000	0.000	67.019	0.000	0.000	0.000	1.767	0.000	0.000	0.000	9582.213
5	4.782	0.000	0.000	0.000	0.000	0.000	6.706	0.000	0.000	0.000	0.000	0.000	0.000	86.146	0.000	0.000	0.000	0.000	0.000	391.069	0.000	0.000	0.000	0.000	0.000	0.000	477.215
6	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	5.264	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	747.672	0.000	0.000	747.672
7	474.596	3.419	0.000	5.264	0.000	0.704	0.000	0.000	0.000	10.558	0.000	0.000	0.000	8549.847	379.401	0.000	716.616	0.000	67.019	0.000	0.000	0.000	617.001	0.000	0.000	0.000	10329.885
8	465.180	3.419	0.000	0.000	0.000	0.704	0.000	0.000	0.000	10.348	0.000	0.000	0.000	8380.225	379.401	0.000	0.000	0.000	67.019	0.000	0.000	0.000	604.760	0.000	0.000	0.000	9431.406
9	9.416	0.000	0.000	5.264	0.000	0.000	0.000	0.000	0.000	0.209	0.000	0.000	0.000	169.622	0.000	0.000	716.616	0.000	0.000	0.000	0.000	0.000	12.241	0.000	0.000	0.000	898.479
10	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	3.419	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	362.338	0.000	362.338
11	465.180	0.000	0.000	0.000	3.419	0.704	0.000	0.000	0.000	17.186	0.000	0.000	0.000	8380.225	0.000	0.000	0.000	342.162	67.019	0.000	0.000	0.000	1004.332	0.000	0.000	0.000	9793.738
12	2.006	0.000	0.000	0.000	3.419	0.704	0.000	0.000	0.000	0.074	0.000	0.000	0.000	36.143	0.000	0.000	0.000	342.162	67.019	0.000	0.000	0.000	4.332	0.000	0.000	0.000	449.656
13	463.174	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	17.112	0.000	0.000	0.000	8344.082	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1000.000	0.000	0.000	0.000	9344.082
14	301.850	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	5437.832	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	5437.832
15	161.324	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	17.112	0.000	0.000	0.000	2906.250	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1000.000	0.000	0.000	0.000	3906.250
16	Boundary flow with impacts assessed through Ecoinvent data set: sodium sulfate production, from natural sources - RoW - sodium sulfate, anhydrite																										N/A
17	Boundary flow with impacts assessed through Ecoinvent data set: soda production, solvay process - RoW - soda ash, light, crystalline, heptahydrate																										
18	Boundary flow with impacts assessed through Ecoinvent data sets: lime production, hydrated, loose weight - RoW - lime, hydrated, loose weight & 'quicklime production, in pieces, loose - RoW - quicklime, in pieces, loose & limestone quarry operation - RoW - limestone, unprocessed																										
19	Boundary flow with impacts assessed through Ecoinvent data set: sodium chloride production, brine solution - RoW - sodium chloride, brine solution																										

Lifecycle Assessment (LCA) Data:

Indicator	Value	Unit
Global Warming Potential (GWP)	2769.551954	kg CO_2-eq. / FU
Ozone Depletion	0.000156	kg CFC-11-eq. / FU
Mineral Resource Depletion	150.379314	kg Cu-eq. / FU
Freshwater Eutrophication Potential	0.460360	kg P-eq. / FU
Marine Eutrophication Potential	1.447138	kg N-eq. / FU
Acidification Potential	8.211096	kg SO_2-eq. / FU
Water Use	11.277094	m^3 / FU

Technoeconomic Assessment (TEA) Data:

Variable	Value	Unit
Purification	0	MJ / FU
Solution Mining	313.19	MJ / FU
Na2SO4 Prod.	611.59	MJ / FU
Na2CO3 Prod.	2721.15	MJ / FU
Ca(OH)2 Prod.	0.69	MJ / FU
CaO Prod.	4.73	MJ / FU
CaCO3 Prod.	14.16	MJ / FU
Evaporator	16912.971	MJ / FU
Total:	20578.50639	MJ / FU

Variable	Value	Unit
Energy Input	20578.50	MJ / FU
Theoretical Energy Requirement	18887.209	MJ / FU
Achieved Energy Efficiency	0.9178	Decimal
Overall Relative Energy Efficiency:	0.9178	Decimal

Variable	Value	Unit
Mass Fed (Total)	11169.44	kg / FU
Mass of Product	1000	kg / FU
Theoretical Maximum Mass Efficiency	0.1827	Decimal
Achieved Mass Efficiency	0.1805	Decimal
Overall Relative Mass Efficiency:	0.9880	Decimal

Flow	Price Data / FU	Data Currency	Year	Price 2022£ / FU:	Quantity Req. (FU):	Total Value:	Unit
Raw Brine	8.5	USD	2022	6.90	0.926	6.39	£ / FU
$Ca(OH)_2$	110	USD	2022	89.27	0.496	44.28	£ / FU
Na_2SO_4	55	USD	2022	44.63	0.362	16.16	£ / FU
Na_2CO_3	360	USD	2022	292.14	0.748	218.52	£ / FU
Natural Gas	0.00578	USD	2022	0.00469	16912.971	79.32	£ / FU
					Total:	366.15	£ / FU

Social Impact Assessment (SIA) Data:

Indicator	Sub-Indicator(s)	Sub-Indicator Value(s)	Final Aggregated Indicator Score
Occupational Health and Safety (OSH)	Accidents causing >4 days' absence	0.689048485	0.611831817
	Work-related disease	0.591438057	
	Work-related mortality	0.582529508	
Child Labour	Non-hazardous	0.769874477	0.607493035
	Hazardous		
	Vulnerability	0.445111594	
Forced Labour	Prevalence	0.941653378	0.693382486
	Vulnerability	0.445111594	
Access to Electricity	Energy imports, net (% of energy use)	0.656944762	0.476854934
	Fossil fuel energy consumption (% of total)	0.264230209	
	Electric power consumption (kWh per capita)	0.01384559	
	Renewable energy consumption (% of total final energy consumption)	0.3293	
Access to Water	Freshwater withdrawal as % of total	0.66115443	0.498116751
	Water Stress	0.335079072	
Land Use Change	-	0.194659486	0.194659486
Utilisation of Hazardous Materials	Deaths caused by dangerous substances per 10,000 workers	0.591436178	0.591436178

Aggregated Final Objective Indicator Scores:

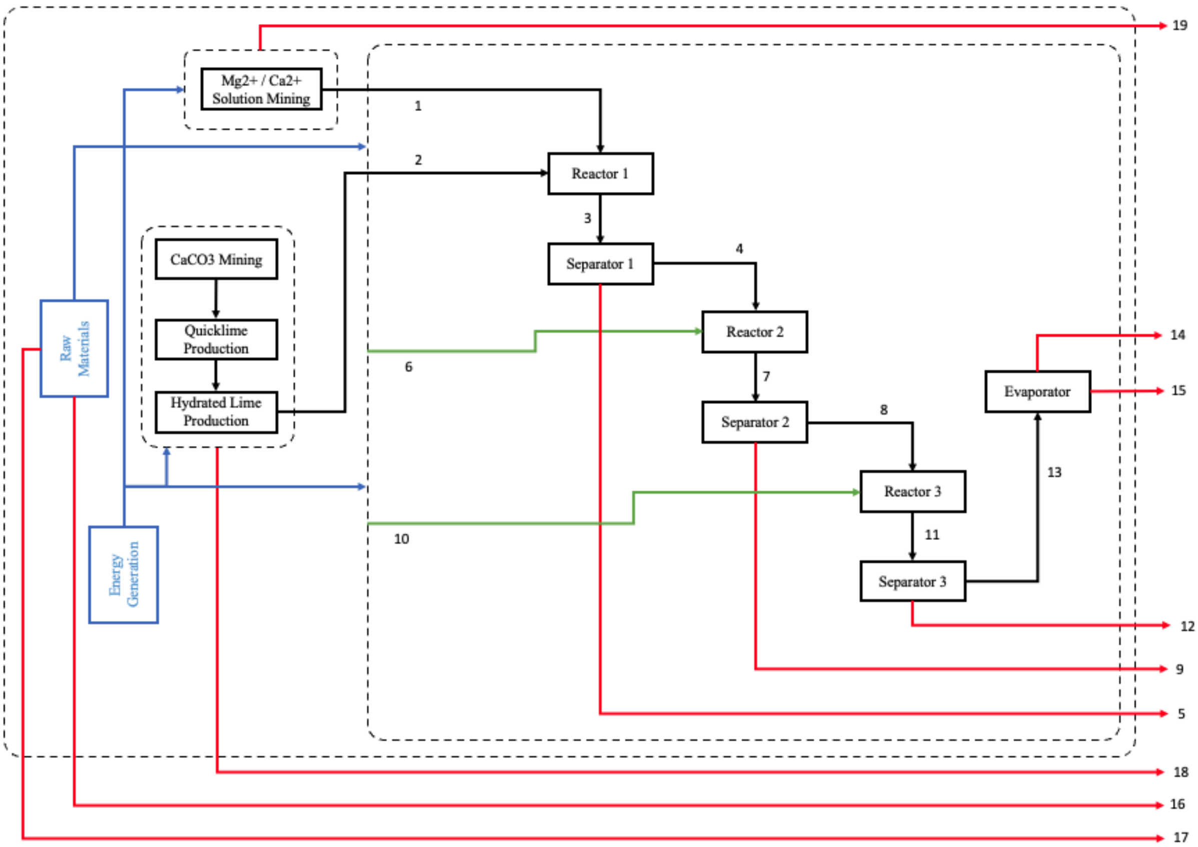
Assessment Strand:	Indicator:	Value:	Units:
LCA	Global Warming Potential (GWP)	2769.551954	kg CO_2-eq. / FU
	Ozone Depletion	0.000156	kg CFC-11-eq. / FU
	Metal Resource Depletion	150.379314	kg Cu-eq. / FU
	Freshwater Eutrophication Potential	0.460360	kg P-eq. / FU
	Marine Eutrophication Potential	1.447138	kg N-eq. / FU
	Acidification Potential	8.211096	kg SO_2-eq. / FU
	Water Use	11.277094	m^3 / FU
TEA	Energy Demand	20578.50639	MJ / FU
	Energy Efficiency (%)	0.9178	%
	Mass Efficiency (%)	0.9880	%
	Est. Purchase Price (2022 £)	366.15	2022 £ / FU
SIA	Occupational Health and Safety (OSH)	0.611831817	-
	Child Labour	0.607493035	-
	Forced Labour	0.693382486	-
	Access to Electricity	0.476854934	-
	Access to Water	0.498116751	-
	Land Use Change	0.194659486	-
	Utilisation of Hazardous Materials	0.591436178	-

Spoke Data Sheet (I.D. 2.4)
(NaCl from Indirect Solution Mining of Mg^{2+} & Ca^{2+} Brine with Ion Exchange and Purification)

Inventory Overview:

Quantity:	Character:
Input or Output?	Input
Reference Flow	1 tonne NaCl via solution mining of Mg^{2+} & Ca^{2+} Brines
Scope	Cradle-to-Gate
Geographic Region	China
Timeframe	2022

System Boundary Block Flow Diagram (BFD):



Spoke Description:

Calcium and magnesium-rich brine is obtained from natural deposits using electrically powered pumping equipment and freshwater. Ecoinvent data is used to quantify the impacts associated with the solution mining (see dataset details in the table below). This solution mining LCI data only covers the extraction process, and it's associated energy, operational, and infrastructure emissions.

Once extracted, the raw brine must be treated to generate NaCl. In this process the brine is treated with $Ca(OH)_2$, Na_2SO_4, and Na_2CO_3 to remove Mg^{2+} ions, Ca^{2+} ions, and the residual Ca^{2+} ions, respectively (see reaction equations below). Using this route, a large proportion of Ca^{2+} ions are deposited in the form of $CaSO_4$ instead of $CaCO_3$, which reduces the soda ash consumption; in addition, $CaSO_4$ and $CaCO_3$ can accelerate further precipitation of $Mg(OH)_2$. After each purification step filters are used to remove solid precipitates.

Equation 0-34

$$MgCl_2 + Ca(OH)_2 \rightarrow Mg(OH)_2 + CaCl_2$$

Equation 0-35

$$Na_2SO_4 + CaCl_2 \rightarrow CaSO_4 + 2NaCl$$

Equation 0-36

$$Na_2CO_3 + CaCl_2 \rightarrow 2NaCl + CaCO_3$$

Na_2SO_4 is obtained through the mining of natural deposits (anhydrous). $Ca(OH)_2$ is obtained through the mining of limestone, it's calcination to form anhydrous quicklime pieces, followed by slaking to produce hydrated lime. Due to the sequential steps in this process, multiple Ecoinvent V3.8 datasets have been aggregated to quantify cradle-to-gate impacts (see details of utilised datasets in the table below). Electricity requirements for the solution mining stage and mining of Na_2SO_4 are reflective of the average European grid mix (a limitation of the Ecoinvent datasets). Heat supplied is based on an Ecoinvent v3.8 data set non-natural gas source, including a mix of; burning biomethane in gas turbine; biogas in co-gen gas engine; anthracite, coal, lignite briquettes and coke in stove; hardwood, logs, softwood, wood chips, wood pellets in furnaces and wood heaters; light fuel oil in boilers. Also contributing are heat from heat pumps and solar collectors. The dataset is targeted for district and industrial-scale heating such as that observed in this system. Additional electricity requirements are evaluated based on the grid mix of the country examined.

After obtaining the NaCl brine, excess water must be evaporated to deliver the required concentration for use in the production of soda ash via the Hou process (25.6 wt%). The heat required for this process is assumed to be delivered through the combustion of natural gas.

Production Step	Dataset / Model Used
Solution mining	Ecoinvent: sodium chloride production, brine solution - RoW - sodium chloride, brine solution
Brine Purification	Brine purification via Na2SO4 and Na2CO3 addition [398] Ecoinvent Supporting Data: 'Soda production, solvay process - RoW - soda ash, light, crystalline, heptahydrate', & 'sodium sulfate production, from natural sources - RoW - sodium sulfate, anhydrite'
Hydrated Lime Production	Ecoinvent Datasets: 'lime production, hydrated, loose weight - RoW - lime, hydrated, loose weight' & 'quicklime production, in pieces, loose - RoW - quicklime, in pieces, loose' & 'limestone quarry operation - RoW - limestone, unprocessed'
Process Heat	Ecoinvent Dataset: 'market for heat, district or industrial, other than natural gas - RoW - heat, district or industrial, other than natural gas'

Boundary Flows:

Classification:	Type:	Description:	Notation:
Input(s)	Raw material extraction	Ecoinvent used to evaluate the impact of feedstock extraction from the environment	N/A
Output(s)	Stream 5	Precipitated $Mg(OH)_2$ from separator 1	5
	Stream 9	Precipitated $CaSO_4$ from separator 2	9
	Stream 12	Precipitated $CaCO_3$ with trace contaminants from separator 3	12
	Stream 14	Water vapour emission from the concentration of brine in the evaporator	14
	Stream15	NaCl brine product	15
	Stream 16	Emissions associated with Na_2SO_4 feedstock production	16
	Stream 17	Emissions associated with Na_2CO_3 feedstock production	17
	Stream 18	Emissions associated with $Ca(OH)_2$ feedstock production	18
	Stream 19	Emissions associated with raw brine (Mg^{2+}/Ca^{2+}) solution mining	19

Process Units Included:

Classification:	Type:	Description:
Primary	Reactor 1	Reaction precipitates magnesium ions in the form of $Mg(OH)_2$ through the addition of $Ca(OH)_2$ to raw brine.
	Reactor 2	Addition of Na_2SO_4 to the remaining raw brine results in the precipitation of calcium ions in the from of $CaSO_4$.
	Reactor 3	Addition of soda ash to brine solution removes any remaining calcium ions in the form of $CaCO_3$.
	Evaporator	The concentration of NaCl to wt% required by the Hou process
Secondary	Separator 1	Removal of the precipitated products of brine purification.
	Separator 2	
	Separator 3	

Assumptions:

Aspect:	Assumption(s):
System Boundary	• Ecoinvent datasets assumed to be reflective of the secondary feedstock production (ReCiPe Midpoint (H) characterisation). A secondary sub-system is defined for the production of hydrated lime ($Ca(OH)_2$) due to the absence of cradle-to-gate LCI data within Ecoinvent. • The Ecoinvent sodium chloride solution mining dataset is used as a proxy for the impacts of calcium and magnesium solution mining. The employed technologies and operating conditions are highly comparable (Paidoussis, 2014). • Raw brine prices are not presented by [398]. Therefore, economic data is retrieved for the market average price of brine in 2022 (U.S. Department of the Interior, 2023) • Economic data for industrial natural gas prices per MJ of natural gas in China is obtained from an IEA Report (International Energy Agency, 2023) • 2022 USD to GBP conversion rate is given as 0.7501 as the year’s average (Exchange Rates UK, 2024)
Mass balance	• Raw brine ion composition is derived from Cao, et al. [398] • Final NaCl brine should achieve 25.6 wt% (Kasikowski, et al., 2004) for use in the Hou process • First purification step exhibits a 90.05% efficiency with respect to magnesium ion utilisation [398]. • Second and third purification step efficiencies assumed to be 100% due to irreversibility, and previous work by Cao, et al. [398]. • Mass efficiency of the system is based on the purification loop and thus utilisation of the Ca^{2+} and Mg^{2+}. This is also reflective of the fact that supply chain data get opaquer as the distance to the overall assessment’s ‘hub’ increases.
Energy balance	• The energy demand of the purification steps involves only the pumping and agitation of liquid and conveying of solids. • Covers the energy demand associated with the extraction and handling of raw materials prior to the purification step. • Energy efficiency of heat provision is assumed to be equal to that of typical industrial furnace and heat exchanger arrangements (90%) (Mickey, 2017).
Waste handling	• Gaseous emissions are directly vented. • Liquid effluents released to waterways
Transportation	• Not included
Miscellaneous	• None

Stream Table:

Stream	Species (kmol/hr)													Species In (kg/hr)													Total
	H2O	CaCl2	Ca(OH)2	CaSO4	CaCO3	MgCl2	Mg(OH)2	MgSO4	4MgCO3.Mg(OH)2.4H2O	NaCl	Na2SO4	Na2CO3	CO2	H2O	CaCl2	Ca(OH)2	CaSO4	CaCO3	MgCl2	Mg(OH)2	MgSO4	4MgCO3.Mg(OH)2.4H2O	NaCl	Na2SO4	Na2CO3	CO2	
1	443.900	1.977	0.000	0.000	0.000	7.410	0.000	0.000	0.000	0.030	0.000	0.000	0.000	7996.856	219.391	0.000	0.000	0.000	705.467	0.000	0.000	0.000	1.767	0.000	0.000	0.000	8923.481
2	35.478	0.000	6.706	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	639.137	0.000	496.819	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1135.956
3	479.378	8.682	0.000	0.000	0.000	0.704	6.706	0.000	0.000	0.030	0.000	0.000	0.000	8635.993	963.579	0.000	0.000	0.000	67.019	391.069	0.000	0.000	1.767	0.000	0.000	0.000	10059.428
4	474.596	8.682	0.000	0.000	0.000	0.704	0.000	0.000	0.000	0.030	0.000	0.000	0.000	8549.847	963.579	0.000	0.000	0.000	67.019	0.000	0.000	0.000	1.767	0.000	0.000	0.000	9582.213
5	4.782	0.000	0.000	0.000	0.000	0.000	6.706	0.000	0.000	0.000	0.000	0.000	0.000	86.146	0.000	0.000	0.000	0.000	0.000	391.069	0.000	0.000	0.000	0.000	0.000	0.000	477.215
6	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	5.264	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	747.672	0.000	0.000	747.672
7	474.596	3.419	0.000	5.264	0.000	0.704	0.000	0.000	0.000	10.558	0.000	0.000	0.000	8549.847	379.401	0.000	716.616	0.000	67.019	0.000	0.000	0.000	617.001	0.000	0.000	0.000	10329.885
8	465.180	3.419	0.000	0.000	0.000	0.704	0.000	0.000	0.000	10.348	0.000	0.000	0.000	8380.225	379.401	0.000	0.000	0.000	67.019	0.000	0.000	0.000	604.760	0.000	0.000	0.000	9431.406
9	9.416	0.000	0.000	5.264	0.000	0.000	0.000	0.000	0.000	0.209	0.000	0.000	0.000	169.622	0.000	0.000	716.616	0.000	0.000	0.000	0.000	0.000	12.241	0.000	0.000	0.000	898.479
10	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	3.419	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	362.338	0.000	362.338
11	465.180	0.000	0.000	0.000	3.419	0.704	0.000	0.000	0.000	17.186	0.000	0.000	0.000	8380.225	0.000	0.000	0.000	342.162	67.019	0.000	0.000	0.000	1004.332	0.000	0.000	0.000	9793.738
12	2.006	0.000	0.000	0.000	3.419	0.704	0.000	0.000	0.000	0.074	0.000	0.000	0.000	36.143	0.000	0.000	0.000	342.162	67.019	0.000	0.000	0.000	4.332	0.000	0.000	0.000	449.656
13	463.174	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	17.112	0.000	0.000	0.000	8344.082	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1000.000	0.000	0.000	0.000	9344.082
14	301.850	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	5437.832	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	5437.832
15	161.324	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	17.112	0.000	0.000	0.000	2906.250	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1000.000	0.000	0.000	0.000	3906.250
16	Boundary flow with impacts assessed through Ecoinvent data set: sodium sulfate production, from natural sources - RoW - sodium sulfate, anhydrite																										N/A
17	Boundary flow with impacts assessed through Ecoinvent data set: soda production, solvay process - RoW - soda ash, light, crystalline, heptahydrate																										
18	Boundary flow with impacts assessed through Ecoinvent data sets: lime production, hydrated, loose weight - RoW - lime, hydrated, loose weight & 'quicklime production, in pieces, loose - RoW - quicklime, in pieces, loose & limestone quarry operation - RoW - limestone, unprocessed																										
19	Boundary flow with impacts assessed through Ecoinvent data set: sodium chloride production, brine solution - RoW - sodium chloride, brine solution																										

Lifecycle Assessment (LCA) Data:

Indicator	Value	Unit
Global Warming Potential (GWP)	2769.551954	kg CO_2-eq. / FU
Ozone Depletion	0.000156	kg CFC-11-eq. / FU
Mineral Resource Depletion	150.379314	kg Cu-eq. / FU
Freshwater Eutrophication Potential	0.460360	kg P-eq. / FU
Marine Eutrophication Potential	1.447138	kg N-eq. / FU
Acidification Potential	8.211096	kg SO_2-eq. / FU
Water Use	11.277094	m^3 / FU

Technoeconomic Assessment (TEA) Data:

Variable	Value	Unit
Purification	0	MJ / FU
Solution Mining	313.19	MJ / FU
Na2SO4 Prod.	611.59	MJ / FU
Na2CO3 Prod.	2721.15	MJ / FU
Ca(OH)2 Prod.	0.69	MJ / FU
CaO Prod.	4.73	MJ / FU
CaCO3 Prod.	14.16	MJ / FU
Evaporator	16912.971	MJ / FU
Total:	20578.50639	MJ / FU

Variable	Value	Unit
Energy Input	20578.50	MJ / FU
Theoretical Energy Requirement	18887.209	MJ / FU
Achieved Energy Efficiency	0.9178	Decimal
Overall Relative Energy Efficiency:	0.9178	Decimal

Variable	Value	Unit
Mass Fed (Total)	11169.44	kg / FU
Mass of Product	1000	kg / FU
Theoretical Maximum Mass Efficiency	0.1827	Decimal
Achieved Mass Efficiency	0.1805	Decimal
Overall Relative Mass Efficiency:	0.9880	Decimal

Flow	Price Data / FU	Data Currency	Year	Price 2022£ / FU:	Quantity Req. (FU):	Total Value:	Unit
Raw Brine	8.5	USD	2022	6.90	0.926	6.39	£ / FU
$Ca(OH)_2$	110	USD	2022	89.27	0.496	44.28	£ / FU
Na_2SO_4	55	USD	2022	44.63	0.362	16.16	£ / FU
Na_2CO_3	360	USD	2022	292.14	0.748	218.52	£ / FU
Natural Gas	0.018	USD	2022	0.0146	16912.971	246.93	£ / FU
					Total:	533.76	£ / FU

Social Impact Assessment (SIA) Data:

Indicator	Sub-Indicator(s)	Sub-Indicator Value(s)	Final Aggregated Indicator Score
Occupational Health and Safety (OSH)	Accidents causing >4 days' absence	0.586213385	0.694329585
	Work-related disease	0.754901847	
	Work-related mortality	0.714012633	
Child Labour	Non-hazardous	0.740585774	0.617058249
	Hazardous		
	Vulnerability	0.493530724	
Forced Labour	Prevalence	0.973555901	0.733543312119765
	Vulnerability	0.493530724	
Access to Electricity	Energy imports, net (% of energy use)	0.849781993	0.491839919
	Fossil fuel energy consumption (% of total)	0.123295692	
	Electric power consumption (kWh per capita)	0.070600891	
	Renewable energy consumption (% of total final energy consumption)	0.1445	
Access to Water	Freshwater withdrawal as % of total	0.791635859	0.679709488
	Water Stress	0.567783117	
Land Use Change	-	0.277838446	0.277838445646095
Utilisation of Hazardous Materials	Deaths caused by dangerous substances per 10,000 workers	0.754900315	0.754900315

Aggregated Final Objective Indicator Scores:

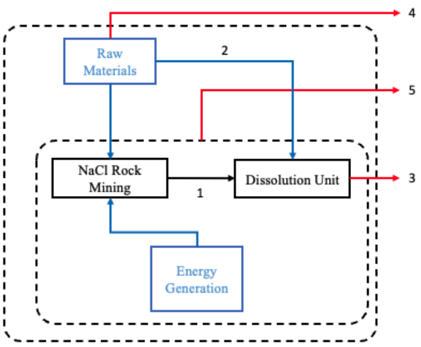
Assessment Strand:	Indicator:	Value:	Units:
LCA	Global Warming Potential (GWP)	2769.551954	kg CO_2-eq. / FU
	Ozone Depletion	0.000156	kg CFC-11-eq. / FU
	Metal Resource Depletion	150.379314	kg Cu-eq. / FU
	Freshwater Eutrophication Potential	0.460360	kg P-eq. / FU
	Marine Eutrophication Potential	1.447138	kg N-eq. / FU
	Acidification Potential	8.211096	kg SO_2-eq. / FU
	Water Use	11.277094	m^3 / FU
TEA	Energy Demand	20578.50639	MJ / FU
	Energy Efficiency (%)	0.9178	%
	Mass Efficiency (%)	0.9880	%
	Est. Purchase Price (2022 £)	533.76	2022 £ / FU
SIA	Occupational Health and Safety (OSH)	0.694329585	-
	Child Labour	0.617058249	-
	Forced Labour	0.733543312	-
	Access to Electricity	0.491839919	-
	Access to Water	0.679709488	-
	Land Use Change	0.277838446	-
	Utilisation of Hazardous Materials	0.754900315	-

Spoke Data Sheet (I.D. 2.5)
(NaCl from Rock Salt Mining)

Inventory Overview:

Quantity:	Character:
Input or Output?	Input
Reference Flow	1 tonne NaCl via rock salt mining
Scope	Cradle-to-Gate
Geographic Region	India
Timeframe	2022

System Boundary Block Flow Diagram (BFD):



Spoke Description:

Rock salt (halite) is the salt left behind by primordial oceans millions of years ago when lagoons dried out. These layers of salt were covered by rock formations and they are now located underground or inside mountains. Rock salt refers to the dry salt extracted from saliferous rock layers with the help of mining methods (Götzfried & Gaudé, 2021). Most salt mines operate underground but in salt deserts, the rock salt is also mined at the surface. Typical underground mining operations are evaluated using Ecoinvent V3.8; The main characteristic of this technique is the fact that salt is not dissolved during the whole process. Instead, underground halite deposits are mined with traditional techniques like undercutting, drilling and blasting or with huge mining machines with cutting heads. In the second step, the salt is crushed and screened to the desired size and then hoisted to the surface (Ecoinvent, 2021). The data used is inclusive of all mine operations and infrastructure development. Mining machinery is electrically driven with emissions based on electricity mixes used in current facilities.

To account for the NaCl feedstock specification for the Hou process (25.6 wt% NaCl brine (Kasikowski, et al., 2004)) the rock salt obtained through mining must be dissolved in water. The impacts of water extraction are accounted for by examining the production of untreated water from the water table using Ecoinvent V3.8. This is then used to dissolve the solid NaCl, producing a sodium brine of the desired concentration.

Boundary Flows:

Classification:	Type:	Description:	Notation:
Input(s)	Raw material extraction	Ecoinvent used to evaluate the impact of feedstock extraction from the environment (water and salt)	N/A
Output(s)	Stream 3	NaCl brine product	3
	Stream 4	Emissions associated with extraction of water for NaCl dissolution	4
	Stream 5	Emissions associated with the construction and operation of the rock salt mine	5

Process Units Included:

Classification:	Type:	Description:
Primary	Rock salt mine	Operation of a rock salt mine producing powdered NaCl
	Dissolution Unit	Mixing of water and solid NaCl to produce brine suitable for the Hou Process

Assumptions:

Aspect:	Assumption(s):
System Boundary	• Ecoinvent datasets assumed to be reflective of the secondary feedstock production (ReCiPe Midpoint (H) characterisation). • Economic data for mined rock salt is based on current industrial supplier prices (Arrow Supplies, 2023) • Economic data for industrial water supply in India is taken as an unweighted average over all states as reported by the Government of India (Dezan Shira & Associates, 2018). • 2018 USD to GBP conversion rate is given as 0.7501 as the year's average (Exchange Rates UK, 2024) • Inflation of 2018 GBP to 2022 GBP utilises a conversion factor of 1.14896 (The Bank of England, 2024)
Mass balance	• Final NaCl brine should achieve 25.6 wt% (Kasikowski, et al., 2004) for use in the Hou process • Dissolution unit assumed to be 100% efficient as saturation limit is not reached • Mass efficiency of the system is based on solely the NaCl dissolution step as the mining efficiency is considered an upstream process.
Energy balance	• Machinery and units are electrically driven, resulting in 100% energy efficiency at this step. • Dissolution unit energy efficiency is assumed to be 80%, in line with design heuristics from Walas, 2002 (Walas, 2002) • Mixing of the fluid within the dissolution unit is assumed to require 2J / kg of liquid for good adequate performance (Berk, 2009)
Waste handling	• Gaseous emissions are directly vented. • Liquid effluents released to waterways
Transportation	• Not included
Miscellaneous	• None

Stream Table:

Stream	Species (kmol/hr)		Species In (kg/hr)		Total
	H2O	NaCl	H2O	NaCl	
1	0	17.11156742	0.000	1000.000	1000.000
2	161.3238968	0	2906.250	0.000	2906.250
3	161.3238968	17.11156742	2906.250	1000.000	3906.250
4	Boundary flow with impacts assessed through Ecoinvent data set: 'tap water production, underground water without treatment - RoW - tap water' Note: This				0.000
5	Boundary flow with impacts assessed through Ecoinvent data set: 'sodium chloride production, powder - RoW - sodium chloride, powder' Note:				0.000

Lifecycle Assessment (LCA) Data:

Indicator	Value	Unit
Global Warming Potential (GWP)	254.884083	kg CO_2-eq. / FU
Ozone Depletion	0.000008	kg CFC-11-eq. / FU
Mineral Resource Depletion	53.864665	kg Cu-eq. / FU
Freshwater Eutrophication Potential	0.154215	kg P-eq. / FU
Marine Eutrophication Potential	0.381845	kg N-eq. / FU
Acidification Potential	1.454617	kg SO_2-eq. / FU
Water Use	3.973870	m^3 / FU

Technoeconomic Assessment (TEA) Data:

Variable	Value	Unit
Rock Salt Mining	201.28	MJ / FU
Dissolution Unit	0.00977	MJ / FU
Total:	201.28977	MJ / FU

Variable	Value	Unit
Energy Input	201.28977	MJ / FU
Theoretical Energy Requirement	201.28782	MJ / FU
Achieved Energy Efficiency	0.9999	Decimal
Overall Relative Energy Efficiency:	0.9999	Decimal

Variable	Value	Unit
Mass Fed (Total)	3906.25	kg / FU
Mass of Product	1000	kg / FU
Theoretical Maximum Mass Efficiency	1	Decimal
Achieved Mass Efficiency	1	Decimal
Overall Relative Mass Efficiency:	1	Decimal

Flow	Price Data / FU	Data Currency	Year	Price 2022£ / FU:	Quantity Req. (FU):	Total Value:	Unit
Mined NaCl	227.85	£	2022	227.85	1	227.85	£ / FU
Water	0.65	$	2018	0.49	2.906	1.42	£ / FU
					Total:	229.27	£ / FU

Social Impact Assessment (SIA) Data:

Indicator	Sub-Indicator(s)	Sub-Indicator Value(s)	Final Aggregated Indicator Score
Occupational Health and Safety (OSH)	Accidents causing >4 days' absence	0.689048485	0.611831817
	Work-related disease	0.591438057	
	Work-related mortality	0.582529508	
Child Labour	Non-hazardous	0.769874477	0.607493035
	Hazardous		
	Vulnerability	0.445111594	
Forced Labour	Prevalence	0.941653378	0.693382486
	Vulnerability	0.445111594	
Access to Electricity	Energy imports, net (% of energy use)	0.656944762	0.476854934
	Fossil fuel energy consumption (% of total)	0.264230209	
	Electric power consumption (kWh per capita)	0.01384559	
	Renewable energy consumption (% of total final energy consumption)	0.3293	
Access to Water	Freshwater withdrawal as % of total	0.66115443	0.498116751
	Water Stress	0.335079072	
Land Use Change	-	0.194659486	0.194659486
Utilisation of Hazardous Materials	Deaths caused by dangerous substances per 10,000 workers	0.591436178	0.591436178

Aggregated Final Objective Indicator Scores:

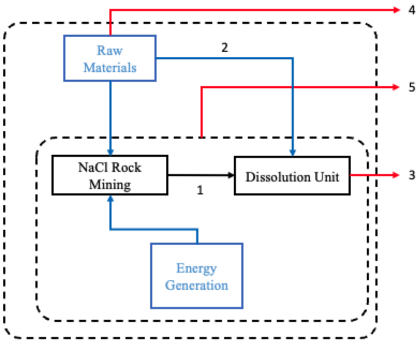
Assessment Strand:	Indicator:	Value:	Units:
LCA	Global Warming Potential (GWP)	254.884083	kg CO_2-eq. / FU
	Ozone Depletion	0.000008	kg CFC-11-eq. / FU
	Metal Resource Depletion	53.864665	kg Cu-eq. / FU
	Freshwater Eutrophication Potential	0.154215	kg P-eq. / FU
	Marine Eutrophication Potential	0.381845	kg N-eq. / FU
	Acidification Potential	1.454617	kg SO_2-eq. / FU
	Water Use	3.973870	m^3 / FU
TEA	Energy Demand	201.28977	MJ / FU
	Energy Efficiency (%)	0.9999	%
	Mass Efficiency (%)	1	%
	Est. Purchase Price (2022 £)	229.27	2022 £ / FU
SIA	Occupational Health and Safety (OSH)	0.611831817	-
	Child Labour	0.607493035	-
	Forced Labour	0.693382486	-
	Access to Electricity	0.476854934	-
	Access to Water	0.498116751	-
	Land Use Change	0.194659486	-
	Utilisation of Hazardous Materials	0.591436178	-

Spoke Data Sheet (I.D, 2.6)
(NaCl from Rock Salt Mining)

Inventory Overview:

Quantity:	Character:
Input or Output?	Input
Reference Flow	1 tonne NaCl via rock salt mining
Scope	Cradle-to-Gate
Geographic Region	China
Timeframe	2022

System Boundary Block Flow Diagram (BFD):



Spoke Description:

Rock salt (halite) is the salt left behind by primordial oceans millions of years ago when lagoons dried out. These layers of salt were covered by rock formations and they are now located underground or inside mountains. Rock salt refers to the dry salt extracted from saliferous rock layers with the help of mining methods (Götzfried & Gaudé, 2021). Most salt mines operate underground but in salt deserts, the rock salt is also mined at the surface. Typical underground mining operations are evaluated using Ecoinvent V3.8; The main characteristic of this technique is the fact that salt is not dissolved during the whole process. Instead, underground halite deposits are mined with traditional techniques like undercutting, drilling and blasting or with huge mining machines with cutting heads. In the second step, the salt is crushed and screened to the desired size and then hoisted to the surface (Ecoinvent, 2021). The data used is inclusive of all mine operations and infrastructure development. Mining machinery is electrically driven with emissions based on electricity mixes used in current facilities.

To account for the NaCl feedstock specification for the Hou process (25.6 wt% NaCl brine (Kasikowski, et al., 2004)) the rock salt obtained through mining must be dissolved in water. The impacts of water extraction are accounted for by examining the production of untreated water from the water table using Ecoinvent V3.8. This is then used to dissolve the solid NaCl, producing a sodium brine of the desired concentration.

Boundary Flows:

Classification:	Type:	Description:	Notation:
Input(s)	Raw material extraction	Ecoinvent used to evaluate the impact of feedstock extraction from the environment (water and salt)	N/A
Output(s)	Stream 3	NaCl brine product	3
	Stream 4	Emissions associated with extraction of water for NaCl dissolution	4
	Stream 5	Emissions associated with the construction and operation of the rock salt mine	5

Process Units Included:

Classification:	Type:	Description:
Primary	Rock salt mine	Operation of a rock salt mine producing powdered NaCl
	Dissolution Unit	Mixing of water and solid NaCl to produce brine suitable for the Hou Process

Assumptions:

Aspect:	Assumption(s):
System Boundary	• Ecoinvent datasets assumed to be reflective of the secondary feedstock production (ReCiPe Midpoint (H) characterisation). • Economic data for mined rock salt is based on current industrial supplier prices (Arrow Supplies, 2023) • Economic data for industrial water supply in China is taken from the literature (Statista, 2023). • 2022 USD to GBP conversion rate is given as 0.7501 as the year's average (Exchange Rates UK, 2024)
Mass balance	• Final NaCl brine should achieve 25.6 wt% (Kasikowski, et al., 2004) for use in the Hou process • Dissolution unit assumed to be 100% efficient as saturation limit is not reached • Mass efficiency of the system is based on solely the NaCl dissolution step as the mining efficiency is considered an upstream process.
Energy balance	• Machinery and units are electrically driven, resulting in 100% energy efficiency at this step. • Dissolution unit energy efficiency is assumed to be 80%, in line with design heuristics from Walas, 2002 (Walas, 2002) • Mixing of the fluid within the dissolution unit is assumed to require 2J / kg of liquid for good adequate performance (Berk, 2009)
Waste handling	• Gaseous emissions are directly vented. • Liquid effluents released to waterways
Transportation	• Not included
Miscellaneous	• None

Stream Table:

Stream	Species (kmol/hr)		Species In (kg/hr)		Total
	H2O	NaCl	H2O	NaCl	
1	0	17.11156742	0.000	1000.000	1000.000
2	161.3238968	0	2906.250	0.000	2906.250
3	161.3238968	17.11156742	2906.250	1000.000	3906.250
4	Boundary flow with impacts assessed through Ecoinvent data set: 'tap water production, underground water without treatment - RoW - tap water' Note: This				0.000
5	Boundary flow with impacts assessed through Ecoinvent data set: 'sodium chloride production, powder - RoW - sodium chloride, powder' Note:				0.000

Lifecycle Assessment (LCA) Data:

Indicator	Value	Unit
Global Warming Potential (GWP)	254.884083	kg CO_2-eq. / FU
Ozone Depletion	0.000008	kg CFC-11-eq. / FU
Mineral Resource Depletion	53.864665	kg Cu-eq. / FU
Freshwater Eutrophication Potential	0.154215	kg P-eq. / FU
Marine Eutrophication Potential	0.381845	kg N-eq. / FU
Acidification Potential	1.454617	kg SO_2-eq. / FU
Water Use	3.973870	m^3 / FU

Technoeconomic Assessment (TEA) Data:

Variable	Value	Unit
Rock Salt Mining	201.28	MJ / FU
Dissolution Unit	0.00977	MJ / FU
Total:	201.28977	MJ / FU

Variable	Value	Unit
Energy Input	201.28977	MJ / FU
Theoretical Energy Requirement	201.28782	MJ / FU
Achieved Energy Efficiency	0.9999	Decimal
Overall Relative Energy Efficiency:	0.9999	Decimal

Variable	Value	Unit
Mass Fed (Total)	3906.25	kg / FU
Mass of Product	1000	kg / FU
Theoretical Maximum Mass Efficiency	1	Decimal
Achieved Mass Efficiency	1	Decimal
Overall Relative Mass Efficiency:	1	Decimal

Flow	Price Data / FU	Data Currency	Year	Price 2022£ / FU:	Quantity Req. (FU):	Total Value:	Unit
Mined NaCl	227.85	£	2022	227.85	1	227.85	£ / FU
Water	0.36	$	2022	0.27	2.906	0.78	£ / FU
					Total:	228.63	£ / FU

Social Impact Assessment (SIA) Data:

Indicator	Sub-Indicator(s)	Sub-Indicator Value(s)	Final Aggregated Indicator Score
Occupational Health and Safety (OSH)	Accidents causing >4 days' absence	0.586213385	0.694329585
	Work-related disease	0.754901847	
	Work-related mortality	0.714012633	
Child Labour	Non-hazardous	0.740585774	0.617058249
	Hazardous		
	Vulnerability	0.493530724	
Forced Labour	Prevalence	0.973555901	0.733543312119765
	Vulnerability	0.493530724	
Access to Electricity	Energy imports, net (% of energy use)	0.849781993	0.491839919
	Fossil fuel energy consumption (% of total)	0.123295692	
	Electric power consumption (kWh per capita)	0.070600891	
	Renewable energy consumption (% of total final energy consumption)	0.1445	
Access to Water	Freshwater withdrawal as % of total	0.791635859	0.679709488
	Water Stress	0.567783117	
Land Use Change	-	0.277838446	0.277838445646095
Utilisation of Hazardous Materials	Deaths caused by dangerous substances per 10,000 workers	0.754900315	0.754900315

Aggregated Final Objective Indicator Scores:

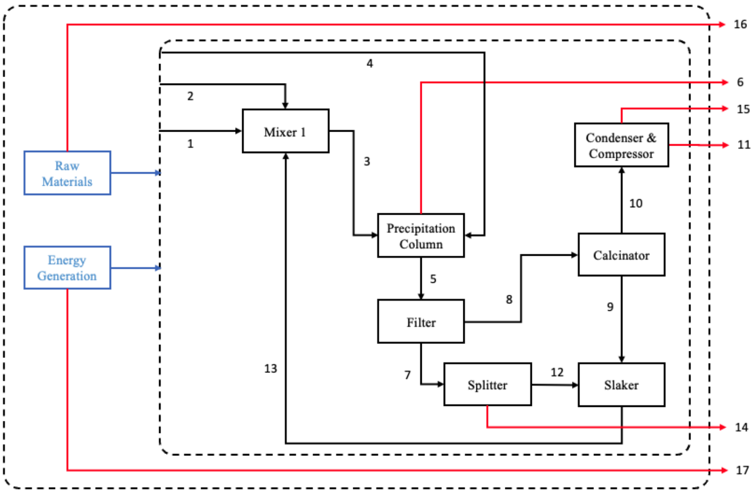
Assessment Strand:	Indicator:	Value:	Units:
LCA	Global Warming Potential (GWP)	254.884083	kg CO_2-eq. / FU
	Ozone Depletion	0.000008	kg CFC-11-eq. / FU
	Metal Resource Depletion	53.864665	kg Cu-eq. / FU
	Freshwater Eutrophication Potential	0.154215	kg P-eq. / FU
	Marine Eutrophication Potential	0.381845	kg N-eq. / FU
	Acidification Potential	1.454617	kg SO_2-eq. / FU
	Water Use	3.973870	m^3 / FU
TEA	Energy Demand	201.28977	MJ / FU
	Energy Efficiency (%)	0.9999	%
	Mass Efficiency (%)	1	%
	Est. Purchase Price (2022 £)	228.63	2022 £ / FU
SIA	Occupational Health and Safety (OSH)	0.694329585	-
	Child Labour	0.617058249	-
	Forced Labour	0.733543312	-
	Access to Electricity	0.491839919	-
	Access to Water	0.679709488	-
	Land Use Change	0.277838446	-
	Utilisation of Hazardous Materials	0.754900315	-

Spoke Data Sheet (I.D. 3.1)
(CO_2 from Direct Air Capture)

Inventory Overview:

Quantity:	Character:
Input or Output?	Input
Reference Flow	1 tonne CO_2 via Direct Air Capture
Scope	Cradle-to-Gate
Geographic Region	India
Timeframe	2022

System Boundary Block Flow Diagram (BFD):



Spoke Description:

Within this spoke dataset, $Ca(OH)_2$ based direct air capture (DAC) of CO_2 is considered. This is one of the original DAC techniques and acts as a 'strawman' for the CO_2 market in terms of performance and cost (Sanz-Pérez, et al., 2016). Due to the ultra-dilute nature of CO_2 in the atmosphere, chemical sorbents with strong CO_2-binding affinities are typically employed for CO2 capture (Sanz-Pérez, et al., 2016). While newer and more technologically advanced processes are present, this method of capture was selected due to the availability of literature and suitability as a meaningful baseline. The advantage of this method is that calcium hydroxide is a low-cost and widely available material. However, challenges include the energy requirements for the regeneration step and the need for efficient separation of the solid calcium carbonate particles. $Ca(OH)_2$ DAC consist of the following reaction steps:

Step	Reaction
1	$Ca(OH)_2 + CO_2 \rightarrow CaCO_3 + H_2O$
2	$CaCO_3 \rightarrow CaO + CO_2$
3	$CaO + H_2O \rightarrow Ca(OH)_2$

The reaction enthalpy of steps 1 and 3 are exothermic, with step 2 having an endothermic energy requirement of 179.2 kJ mol^{-1} (Sanz-Pérez, et al., 2016). To maintain an assessment scenario equitable to that of MEA-based capture, heat integration from the exothermic steps is not considered. Furthermore, to reflect real deployment scenarios, natural gas heating will be used to provide the energy required in step 2. Additional energy requirements will be met via the grid mix of the considered country. Impacts associated with top-up lime and water production are quantified using Ecoinvent v3.8 ('lime production, hydraulic - RoW - lime, hydraulic'). Atmospheric concentrations are treated as globally uniform, with composition detailed in the table below.

Air Composition		
Component	Percentage Presence	Unit
N_2	78.08	%
O_2	20.95	%
Argon	0.93	%
CO_2	0.04	%

Boundary Flows:

Classification:	Type:	Description:	Notation:
Input(s)	Raw material extraction	Ecoinvent used to evaluate the impact of feedstock extraction from the environment	N/A
	Stream 1 (Air)	Assumed free of burden and cost	1
Output(s)	Stream 6	CO_2 free air	6
	Stream 11	CO_2 product stream	11
	Stream 14	Water purge (with low concentrations of $Ca(OH)_2$) to prevent recycle loop accumulation.	14
	Stream 15	Waste stream (water) from CO_2 condensation and compression	15
	Stream 16	Emissions associated with extraction and preparation of the required feedstocks	16
	Stream 17	Emissions associated with generation of the required energy (electrical and heat)	17

Process Units Included:

Classification:	Type:	Description:
Primary	Precipitation Column	Capture of CO2 via reaction with $Ca(OH)_2$ and precipitation as $CaCO_3$.
	Calcinator	Thermal decomposition of precipitated $CaCO_3$, forming CaO, and CO_2.
	Slaker	Hydration of CaO to generate $Ca(OH)_2$ for recycle to the precipitation column.
Secondary	Mixer	Mixes water and CaO top-up stream with the recycle stream (13).
	Filter	Separates precipitated $CaCO_3$ from the liquid outlet of the distillation column.
	Splitter	Removes water from the recycle loop to prevent accumulation origination from the water released through reaction in the precipitation column.
	Condenser	Separates water and CO_2 from the calcinator based on boiling point
	Compressor	Compression of CO_2 to achieve liquid state

Assumptions:

Aspect:	Assumption(s):
System Boundary	• Ecoinvent datasets assumed to be reflective of the secondary feedstock production (ReCiPe Midpoint (H) characterisation) • Atmospheric air assumed to be free of burden and cost. • CO_2 removed from air is evaluated as a negative emission. • Electricity generation is handled via the national grid mix of the considered country. • Heat is supplied via methane combustion. ○ Mol/m^3 supplied is evaluated using ideal gas law (5 Bar, 298.15 K) • Cost estimation of \$1000/tonne is taken from a comparable system in literature (House, et al., 2011). • 2011 USD to GBP conversion rate is given as 0.6236 as the year's average (Exchange Rates UK, 2024) • Inflation of 2011 GBP to 2022 GBP utilises a conversion factor of 1.30279 (The Bank of England, 2024)
Mass balance	• Composition of ambient air taken from literature (NASA, 2019) • Filters assumed to be 100% efficient. • 10% excess $Ca(OH)_2$ feed to precipitation column (ensures completion & top-up not affected due to recycle) • $Ca(OH)_2$ feed is at saturation assuming 20ºC at 1 atm (0. 0.0004597 mol $Ca(OH)_2$ / mol H_2O) (Rumble, 2018) • Emissions calculations from methane combustion for steam generation assume an optimal 90% combustion efficiency (Mickey, 2017) and 84.3% heat recovery (Najmi & Arhosazni, 2006)
Energy balance	• Compression of CO_2 product stream (ambient to liquid) requires 110 kWh per tonne as per literature examining a CCS plant (Jackson & Brodal, 2018). • Latent heat of water taken as 2,260 kJ / kg (Datt, 2011) • Specific heat capacity of water taken as a constant over the temperature range examined and determined to be 4.2 kJ / kgK (Desmos, 2023). • Calcinator energy requirement is inclusive of the entrained water within the filter cake.
Waste handling	• Gaseous emissions are directly vented. • Liquid effluents released to waterways
Transportation	• Not included
Miscellaneous	• None

Stream Table:

Stream	Species (kmol/hr)								Species (kg/hr)								Total
	N_2	O_2	Ar	CO_2	$Ca(OH)_2$	$CaCO_3$	CaO	H_2O	N_2	O_2	Ar	CO_2	$Ca(OH)_2$	$CaCO_3$	CaO	H_2O	
1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	77.13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1388.39	1388.39
2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.18	0.00	0.18
3	0.00	0.00	0.00	0.00	25.00	0.00	0.00	54379.78	0.00	0.00	0.00	0.00	1850.00	0.00	0.00	978835.98	980685.98
4	44363.64	11903.41	528.41	22.73	0.00	0.00	0.00	0.00	1242181.82	380909.09	21136.36	1000.00	0.00	0.00	0.00	0.00	1645227.27
5	0.00	0.00	0.00	0.00	2.27	22.73	0.00	54402.50	0.00	0.00	0.00	0.00	168.18	2272.73	0.00	979245.07	981685.98
6	44363.64	11903.41	528.41	0.00	0.00	0.00	0.00	0.00	1242181.82	380909.09	21136.36	0.00	0.00	0.00	0.00	0.00	1644227.27
7	0.00	0.00	0.00	0.00	2.27	0.00	0.00	54348.10	0.00	0.00	0.00	0.00	168.01	0.00	0.00	978265.82	978433.84
8	0.00	0.00	0.00	0.00	0.00	22.73	0.00	54.40	0.00	0.00	0.00	0.00	0.17	2272.73	0.00	979.25	3252.14
9	0.00	0.00	0.00	0.00	0.00	0.00	22.73	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1272.73	0.00	1272.73
10	0.00	0.00	0.00	22.73	0.00	0.00	0.00	54.40	0.00	0.00	0.00	1000.00	0.00	0.00	0.00	979.25	1979.25
11	0.00	0.00	0.00	22.73	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1000.00	0.00	0.00	0.00	0.00	1000.00
12	0.00	0.00	0.00	0.00	2.27	0.00	0.00	54325.37	0.00	0.00	0.00	0.00	167.94	0.00	0.00	977856.73	978024.68
13	0.00	0.00	0.00	0.00	25.00	0.00	0.00	54302.65	0.00	0.00	0.00	0.00	1849.76	0.00	0.00	977447.64	979297.40
14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	22.73	0.00	0.00	0.00	0.00	0.07	0.00	0.00	409.09	409.16
15	0.00	0.00	0.00	0.00	0.00	0.00	0.00	54.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00	979.25	979.25
16	Boundary flow with impacts assessed through Ecoinvent data set: 'lime production, hydraulic - RoW - lime, hydraulic' & 'tap water production, underground water without treatment - RoW - tap water'																N/A
17	Boundary flow with impacts assessed through Ecoinvent data set: 'natural gas production - US - natural gas, high pressure' & stochiometric evaluation of emissions (CH4 & CO2)																

Lifecycle Assessment (LCA) Data:

Indicator	Value	Unit
Global Warming Potential (GWP)	-150.521966	kg CO_2-eq. / FU
Ozone Depletion	0.000001	kg CFC-11-eq. / FU
Metal Resource Depletion	1.188328	kg Cu-eq. / FU
Freshwater Eutrophication Potential	0.082796	kg P-eq. / FU
Marine Eutrophication Potential	0.136841	kg N-eq. / FU
Acidification Potential	0.751814	kg SO_2-eq. / FU
Water Use	1.803762	m^3 / FU

Technoeconomic Assessment (TEA) Data

Variable	Value	Unit
$CaCO_3$ calcination	4072.73	MJ / FU
Water evaporation during calcination	2459.86	MJ / FU
CO_2 compression	396	MJ / FU
Total:	6928.59	MJ / FU

Variable	Value	Unit
Energy Input	6928.59	MJ / FU
Theoretical Energy Requirement	6275.331	MJ / FU
Achieved Energy Efficiency	0.9057	Decimal
Overall Relative Energy Efficiency:	0.9057	Decimal

Variable	Value	Unit
Mass Fed (Total)	1646615.85	kg / FU
Mass of Product	1000	kg / FU
Theoretical Maximum Mass Efficiency	1	Decimal
Achieved Mass Efficiency	1	Decimal
Overall Relative Mass Efficiency:	1	Decimal

Flow	Price Data / FU	Data Currency	Year	Price 2022£ / FU:	Quantity Req. (FU):	Total Value:	Unit
Liquified CO_2 from $Ca(OH)_2$ based DAC	1000	USD	2011	812.42	1	812.42	£ / FU
					Total:	812.42	£ / FU

Social Impact Assessment (SIA) Data:

Indicator	Sub-Indicator(s)	Sub-Indicator Value(s)	Final Aggregated Indicator Score
Occupational Health and Safety (OSH)	Accidents causing >4 days' absence	0.689048485	0.611831817
	Work-related disease	0.591438057	
	Work-related mortality	0.582529508	
Child Labour	Non-hazardous	0.769874477	0.607493035
	Hazardous		
	Vulnerability	0.445111594	
Forced Labour	Prevalence	0.941653378	0.693382486
	Vulnerability	0.445111594	
Access to Electricity	Energy imports, net (% of energy use)	0.656944762	0.476854934
	Fossil fuel energy consumption (% of total)	0.264230209	
	Electric power consumption (kWh per capita)	0.01384559	
	Renewable energy consumption (% of total final energy consumption)	0.3293	
Access to Water	Freshwater withdrawal as % of total	0.66115443	0.498116751
	Water Stress	0.335079072	
Land Use Change	-	0.194659486	0.194659486
Utilisation of Hazardous Materials	Deaths caused by dangerous substances per 10,000 workers	0.591436178	0.591436178

Aggregated Final Objective Indicator Scores:

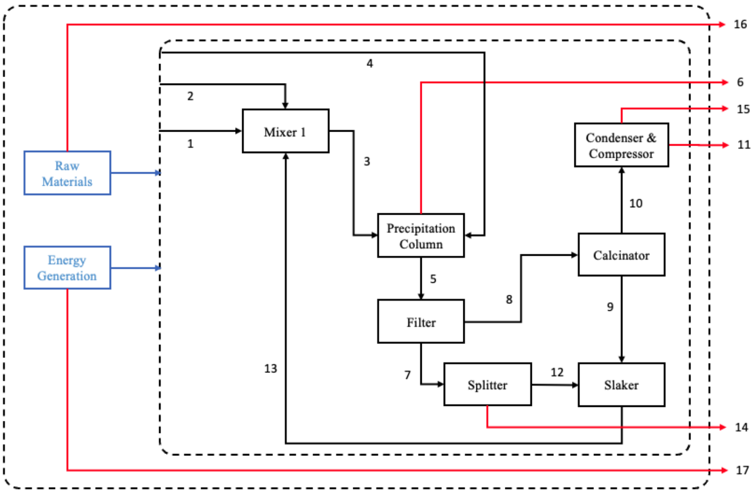
Assessment Strand:	Indicator:	Value:	Units:
LCA	Global Warming Potential (GWP)	-150.521966	kg CO_2-eq. / FU
	Ozone Depletion	0.000001	kg CFC-11-eq. / FU
	Metal Resource Depletion	1.188328	kg Cu-eq. / FU
	Freshwater Eutrophication Potential	0.082796	kg P-eq. / FU
	Marine Eutrophication Potential	0.136841	kg N-eq. / FU
	Acidification Potential	0.751814	kg SO_2-eq. / FU
	Water Use	1.803762	m^3 / FU
TEA	Energy Demand	6928.59	MJ / FU
	Energy Efficiency (%)	0.9057	%
	Mass Efficiency (%)	1	%
	Est. Purchase Price (2022 £)	812.42	2022 £ / FU
SIA	Occupational Health and Safety (OSH)	0.611831817	-
	Child Labour	0.607493035	-
	Forced Labour	0.693382486	-
	Access to Electricity	0.476854934	-
	Access to Water	0.498116751	-
	Land Use Change	0.194659486	-
	Utilisation of Hazardous Materials	0.591436178	-

Spoke Data Sheet (I.D. 3.2)
(CO_2 from Direct Air Capture)

Inventory Overview:

Quantity:	Character:
Input or Output?	Input
Reference Flow	1 tonne CO_2 via Direct Air Capture
Scope	Cradle-to-Gate
Geographic Region	China
Timeframe	2022

System Boundary Block Flow Diagram (BFD):



Spoke Description:

Within this spoke dataset, $Ca(OH)_2$ based direct air capture (DAC) of CO_2 is considered. This is one of the original DAC techniques and acts as a 'strawman' for the CO_2 market in terms of performance and cost (Sanz-Pérez, et al., 2016). Due to the ultra-dilute nature of CO_2 in the atmosphere, chemical sorbents with strong CO_2-binding affinities are typically employed for CO2 capture (Sanz-Pérez, et al., 2016). While newer and more technologically advanced processes are present, this method of capture was selected due to the availability of literature and suitability as a meaningful baseline. The advantage of this method is that calcium hydroxide is a low-cost and widely available material. However, challenges include the energy requirements for the regeneration step and the need for efficient separation of the solid calcium carbonate particles. $Ca(OH)_2$ DAC consist of the following reaction steps:

Step	Reaction
1	$Ca(OH)_2 + CO_2 \rightarrow CaCO_3 + H_2O$
2	$CaCO_3 \rightarrow CaO + CO_2$
3	$CaO + H_2O \rightarrow Ca(OH)_2$

The reaction enthalpy of steps 1 and 3 are exothermic, with step 2 having an endothermic energy requirement of 179.2 kJ mol^{-1} (Sanz-Pérez, et al., 2016). To maintain an assessment scenario equitable to that of MEA-based capture, heat integration from the exothermic steps is not considered. Furthermore, to reflect real deployment scenarios, natural gas heating will be used to provide the energy required in step 2. Additional energy requirements will be met via the grid mix of the considered country. Impacts associated with top-up lime and water production are quantified using Ecoinvent v3.8 ('lime production, hydraulic - RoW - lime, hydraulic'). Atmospheric concentrations are treated as globally uniform, with composition detailed in the table below.

Air Composition		
Component	Percentage Presence	Unit
N_2	78.08	%
O_2	20.95	%
Argon	0.93	%
CO_2	0.04	%

Boundary Flows:

Classification:	Type:	Description:	Notation:
Input(s)	Raw material extraction	Ecoinvent used to evaluate the impact of feedstock extraction from the environment	N/A
	Stream 1 (Air)	Assumed free of burden and cost	1
Output(s)	Stream 6	CO_2 free air	6
	Stream 11	CO_2 product stream	11
	Stream 14	Water purge (with low concentrations of $Ca(OH)_2$) to prevent recycle loop accumulation.	14
	Stream 15	Waste stream (water) from CO_2 condensation and compression	15
	Stream 16	Emissions associated with extraction and preparation of the required feedstocks	16
	Stream 17	Emissions associated with generation of the required energy (electrical and heat)	17

Process Units Included:

Classification:	Type:	Description:
Primary	Precipitation Column	Capture of CO2 via reaction with $Ca(OH)_2$ and precipitation as $CaCO_3$.
	Calcinator	Thermal decomposition of precipitated $CaCO_3$, forming CaO, and CO_2.
	Slaker	Hydration of CaO to generate $Ca(OH)_2$ for recycle to the precipitation column.
Secondary	Mixer	Mixes water and CaO top-up stream with the recycle stream (13).
	Filter	Separates precipitated $CaCO_3$ from the liquid outlet of the distillation column.
	Splitter	Removes water from the recycle loop to prevent accumulation origination from the water released through reaction in the precipitation column.
	Condenser	Separates water and CO_2 from the calcinator based on boiling point
	Compressor	Compression of CO_2 to achieve liquid state

Assumptions:

Aspect:	Assumption(s):
System Boundary	• Ecoinvent datasets assumed to be reflective of the secondary feedstock production (ReCiPe Midpoint (H) characterisation) • Atmospheric air assumed to be free of burden and cost. • CO_2 removed from air is evaluated as a negative emission. • Electricity generation is handled via the national grid mix of the considered country. • Heat is supplied via methane combustion. ○ Mol/m^3 supplied is evaluated using ideal gas law (5 Bar, 298.15 K) • Cost estimation of \$1000/tonne is taken from a comparable system in literature (House, et al., 2011). • 2011 USD to GBP conversion rate is given as 0.6236 as the year's average (Exchange Rates UK, 2024) • Inflation of 2011 GBP to 2022 GBP utilises a conversion factor of 1.30279 (The Bank of England, 2024)
Mass balance	• Composition of ambient air taken from literature (NASA, 2019) • Filters assumed to be 100% efficient. • 10% excess $Ca(OH)_2$ feed to precipitation column (ensures completion & top-up not affected due to recycle) • $Ca(OH)_2$ feed is at saturation assuming 20ºC at 1 atm (0. 0.0004597 mol $Ca(OH)_2$ / mol H_2O) (Rumble, 2018) • Emissions calculations from methane combustion for steam generation assume an optimal 90% combustion efficiency (Mickey, 2017) and 84.3% heat recovery (Najmi & Arhosazni, 2006)
Energy balance	• Compression of CO_2 product stream (ambient to liquid) requires 110 kWh per tonne as per literature examining a CCS plant (Jackson & Brodal, 2018). • Latent heat of water taken as 2,260 kJ / kg (Datt, 2011) • Specific heat capacity of water taken as a constant over the temperature range examined and determined to be 4.2 kJ / kgK (Desmos, 2023). • Calcinator energy requirement is inclusive of the entrained water within the filter cake.
Waste handling	• Gaseous emissions are directly vented. • Liquid effluents released to waterways
Transportation	• Not included
Miscellaneous	• None

Stream Table:

Stream	Species (kmol/hr)								Species (kg/hr)								Total
	N_2	O_2	Ar	CO_2	$Ca(OH)_2$	$CaCO_3$	CaO	H_2O	N_2	O_2	Ar	CO_2	$Ca(OH)_2$	$CaCO_3$	CaO	H_2O	
1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	77.13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1388.39	1388.39
2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.18	0.00	0.18
3	0.00	0.00	0.00	0.00	25.00	0.00	0.00	54379.78	0.00	0.00	0.00	0.00	1850.00	0.00	0.00	978835.98	980685.98
4	44363.64	11903.41	528.41	22.73	0.00	0.00	0.00	0.00	1242181.82	380909.09	21136.36	1000.00	0.00	0.00	0.00	0.00	1645227.27
5	0.00	0.00	0.00	0.00	2.27	22.73	0.00	54402.50	0.00	0.00	0.00	0.00	168.18	2272.73	0.00	979245.07	981685.98
6	44363.64	11903.41	528.41	0.00	0.00	0.00	0.00	0.00	1242181.82	380909.09	21136.36	0.00	0.00	0.00	0.00	0.00	1644227.27
7	0.00	0.00	0.00	0.00	2.27	0.00	0.00	54348.10	0.00	0.00	0.00	0.00	168.01	0.00	0.00	978265.82	978433.84
8	0.00	0.00	0.00	0.00	0.00	22.73	0.00	54.40	0.00	0.00	0.00	0.00	0.17	2272.73	0.00	979.25	3252.14
9	0.00	0.00	0.00	0.00	0.00	0.00	22.73	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1272.73	0.00	1272.73
10	0.00	0.00	0.00	22.73	0.00	0.00	0.00	54.40	0.00	0.00	0.00	1000.00	0.00	0.00	0.00	979.25	1979.25
11	0.00	0.00	0.00	22.73	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1000.00	0.00	0.00	0.00	0.00	1000.00
12	0.00	0.00	0.00	0.00	2.27	0.00	0.00	54325.37	0.00	0.00	0.00	0.00	167.94	0.00	0.00	977856.73	978024.68
13	0.00	0.00	0.00	0.00	25.00	0.00	0.00	54302.65	0.00	0.00	0.00	0.00	1849.76	0.00	0.00	977447.64	979297.40
14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	22.73	0.00	0.00	0.00	0.00	0.07	0.00	0.00	409.09	409.16
15	0.00	0.00	0.00	0.00	0.00	0.00	0.00	54.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00	979.25	979.25
16	Boundary flow with impacts assessed through Ecoinvent data set: 'lime production, hydraulic - RoW - lime, hydraulic' & 'tap water production, underground water without treatment - RoW - tap water'																N/A
17	Boundary flow with impacts assessed through Ecoinvent data set: 'natural gas production - US - natural gas, high pressure' & stochiometric evaluation of emissions (CH4 & CO2)																

Lifecycle Assessment (LCA) Data:

Indicator	Value	Unit
Global Warming Potential (GWP)	-164.442211	kg CO_2-eq. / FU
Ozone Depletion	0.000001	kg CFC-11-eq. / FU
Metal Resource Depletion	1.243949	kg Cu-eq. / FU
Freshwater Eutrophication Potential	0.075827	kg P-eq. / FU
Marine Eutrophication Potential	0.117946	kg N-eq. / FU
Acidification Potential	0.642264	kg SO_2-eq. / FU
Water Use	1.753836	m^3 / FU

Technoeconomic Assessment (TEA) Data:

Variable	Value	Unit
$CaCO_3$ calcination	4072.73	MJ / FU
Water evaporation during calcination	2459.86	MJ / FU
CO_2 compression	396	MJ / FU
Total:	6928.59	MJ / FU

Variable	Value	Unit
Energy Input	6928.59	MJ / FU
Theoretical Energy Requirement	6275.331	MJ / FU
Achieved Energy Efficiency	0.9057	Decimal
Overall Relative Energy Efficiency:	0.9057	Decimal

Variable	Value	Unit
Mass Fed (Total)	1646615.85	kg / FU
Mass of Product	1000	kg / FU
Theoretical Maximum Mass Efficiency	1	Decimal
Achieved Mass Efficiency	1	Decimal
Overall Relative Mass Efficiency:	1	Decimal

Flow	Price Data / FU	Data Currency	Year	Price 2022£ / FU:	Quantity Req. (FU):	Total Value:	Unit
Liquified CO_2 from $Ca(OH)_2$ based DAC	1000	USD	2011	812.42	1	812.42	£ / FU
					Total:	812.42	£ / FU

Social Impact Assessment (SIA) Data:

Indicator	Sub-Indicator(s)	Sub-Indicator Value(s)	Final Aggregated Indicator Score
Occupational Health and Safety (OSH)	Accidents causing >4 days' absence	0.586213385	0.694329585
	Work-related disease	0.754901847	
	Work-related mortality	0.714012633	
Child Labour	Non-hazardous	0.740585774	0.617058249
	Hazardous		
	Vulnerability	0.493530724	
Forced Labour	Prevalence	0.973555901	0.733543312
	Vulnerability	0.493530724	
Access to Electricity	Energy imports, net (% of energy use)	0.849781993	0.491839919
	Fossil fuel energy consumption (% of total)	0.123295692	
	Electric power consumption (kWh per capita)	0.070600891	
	Renewable energy consumption (% of total final energy consumption)	0.1445	
Access to Water	Freshwater withdrawal as % of total	0.791635859	0.679709488
	Water Stress	0.567783117	
Land Use Change	-	0.277838446	0.277838446
Utilisation of Hazardous Materials	Deaths caused by dangerous substances per 10,000 workers	0.754900315	0.754900315

Aggregated Final Objective Indicator Scores:

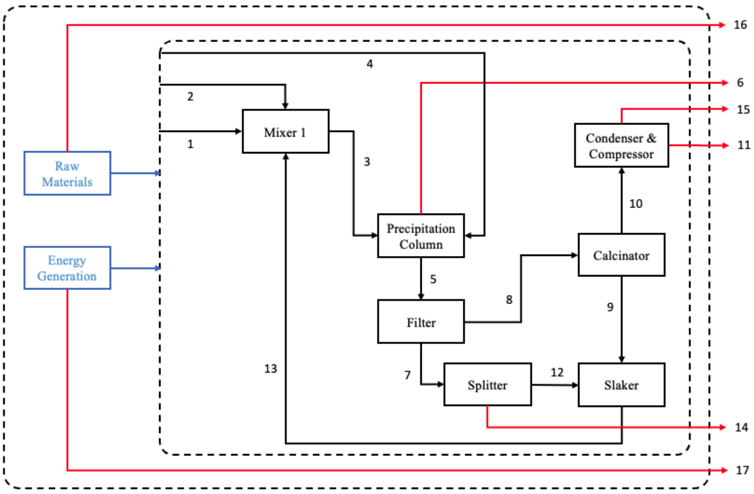
Assessment Strand:	Indicator:	Value:	Units:
LCA	Global Warming Potential (GWP)	-164.442211	kg CO_2-eq. / FU
	Ozone Depletion	0.000001	kg CFC-11-eq. / FU
	Metal Resource Depletion	1.243949	kg Cu-eq. / FU
	Freshwater Eutrophication Potential	0.075827	kg P-eq. / FU
	Marine Eutrophication Potential	0.117946	kg N-eq. / FU
	Acidification Potential	0.642264	kg SO_2-eq. / FU
	Water Use	1.753836	m^3 / FU
TEA	Energy Demand	6928.59	MJ / FU
	Energy Efficiency (%)	0.9057	%
	Mass Efficiency (%)	1	%
	Est. Purchase Price (2022 £)	812.42	2022 £ / FU
SIA	Occupational Health and Safety (OSH)	0.694329585	-
	Child Labour	0.617058249	-
	Forced Labour	0.733543312	-
	Access to Electricity	0.491839919	-
	Access to Water	0.679709488	-
	Land Use Change	0.277838446	-
	Utilisation of Hazardous Materials	0.754900315	-

Spoke Data Sheet (I.D. 3.3)
(CO_2 from Direct Air Capture)

Inventory Overview:

Quantity:	Character:
Input or Output?	Input
Reference Flow	1 tonne CO_2 via Direct Air Capture
Scope	Cradle-to-Gate
Geographic Region	Germany
Timeframe	2022

System Boundary Block Flow Diagram (BFD):



Spoke Description:

Within this spoke dataset, $Ca(OH)_2$ based direct air capture (DAC) of CO_2 is considered. This is one of the original DAC techniques and acts as a 'strawman' for the CO_2 market in terms of performance and cost (Sanz-Pérez, et al., 2016). Due to the ultra-dilute nature of CO_2 in the atmosphere, chemical sorbents with strong CO_2-binding affinities are typically employed for CO2 capture (Sanz-Pérez, et al., 2016). While newer and more technologically advanced processes are present, this method of capture was selected due to the availability of literature and suitability as a meaningful baseline. The advantage of this method is that calcium hydroxide is a low-cost and widely available material. However, challenges include the energy requirements for the regeneration step and the need for efficient separation of the solid calcium carbonate particles. $Ca(OH)_2$ DAC consist of the following reaction steps:

Step	Reaction
1	$Ca(OH)_2 + CO_2 \rightarrow CaCO_3 + H_2O$
2	$CaCO_3 \rightarrow CaO + CO_2$
3	$CaO + H_2O \rightarrow Ca(OH)_2$

The reaction enthalpy of steps 1 and 3 are exothermic, with step 2 having an endothermic energy requirement of 179.2 kJ mol^{-1} (Sanz-Pérez, et al., 2016). To maintain an assessment scenario equitable to that of MEA-based capture, heat integration from the exothermic steps is not considered. Furthermore, to reflect real deployment scenarios, natural gas heating will be used to provide the energy required in step 2. Additional energy requirements will be met via the grid mix of the considered country. Impacts associated with top-up lime and water production are quantified using Ecoinvent v3.8 ('lime production, hydraulic - RoW - lime, hydraulic'). Atmospheric concentrations are treated as globally uniform, with composition detailed in the table below.

Air Composition		
Component	Percentage Presence	Unit
N_2	78.08	%
O_2	20.95	%
Argon	0.93	%
CO_2	0.04	%

Boundary Flows:

Classification:	Type:	Description:	Notation:
Input(s)	Raw material extraction	Ecoinvent used to evaluate the impact of feedstock extraction from the environment	N/A
	Stream 1 (Air)	Assumed free of burden and cost	1
Output(s)	Stream 6	CO_2 free air	6
	Stream 11	CO_2 product stream	11
	Stream 14	Water purge (with low concentrations of $Ca(OH)_2$) to prevent recycle loop accumulation.	14
	Stream 15	Waste stream (water) from CO_2 condensation and compression	15
	Stream 16	Emissions associated with extraction and preparation of the required feedstocks	16
	Stream 17	Emissions associated with generation of the required energy (electrical and heat)	17

Process Units Included:

Classification:	Type:	Description:
Primary	Precipitation Column	Capture of CO2 via reaction with $Ca(OH)_2$ and precipitation as $CaCO_3$.
	Calcinator	Thermal decomposition of precipitated $CaCO_3$, forming CaO, and CO_2.
	Slaker	Hydration of CaO to generate $Ca(OH)_2$ for recycle to the precipitation column.
Secondary	Mixer	Mixes water and CaO top-up stream with the recycle stream (13).
	Filter	Separates precipitated $CaCO_3$ from the liquid outlet of the distillation column.
	Splitter	Removes water from the recycle loop to prevent accumulation origination from the water released through reaction in the precipitation column.
	Condenser	Separates water and CO_2 from the calcinator based on boiling point
	Compressor	Compression of CO_2 to achieve liquid state

Assumptions:

Aspect:	Assumption(s):
System Boundary	• Ecoinvent datasets assumed to be reflective of the secondary feedstock production (ReCiPe Midpoint (H) characterisation) • Atmospheric air assumed to be free of burden and cost. • CO_2 removed from air is evaluated as a negative emission. • Electricity generation is handled via the national grid mix of the considered country. • Heat is supplied via methane combustion. ○ Mol/m^3 supplied is evaluated using ideal gas law (5 Bar, 298.15 K) • Cost estimation of \$1000/tonne is taken from a comparable system in literature (House, et al., 2011). • 2011 USD to GBP conversion rate is given as 0.6236 as the year's average (Exchange Rates UK, 2024) • Inflation of 2011 GBP to 2022 GBP utilises a conversion factor of 1.30279 (The Bank of England, 2024)
Mass balance	• Composition of ambient air taken from literature (NASA, 2019) • Filters assumed to be 100% efficient. • 10% excess $Ca(OH)_2$ feed to precipitation column (ensures completion & top-up not affected due to recycle) • $Ca(OH)_2$ feed is at saturation assuming 20ºC at 1 atm (0. 0.0004597 mol $Ca(OH)_2$ / mol H_2O) (Rumble, 2018) • Emissions calculations from methane combustion for steam generation assume an optimal 90% combustion efficiency (Mickey, 2017) and 84.3% heat recovery (Najmi & Arhosazni, 2006)
Energy balance	• Compression of CO_2 product stream (ambient to liquid) requires 110 kWh per tonne as per literature examining a CCS plant (Jackson & Brodal, 2018). • Latent heat of water taken as 2,260 kJ / kg (Datt, 2011) • Specific heat capacity of water taken as a constant over the temperature range examined and determined to be 4.2 kJ / kgK (Desmos, 2023). • Calcinator energy requirement is inclusive of the entrained water within the filter cake.
Waste handling	• Gaseous emissions are directly vented. • Liquid effluents released to waterways
Transportation	• Not included
Miscellaneous	• None

Stream Table:

Stream	Species (kmol/hr)								Species (kg/hr)								Total
	N_2	O_2	Ar	CO_2	$Ca(OH)_2$	$CaCO_3$	CaO	H_2O	N_2	O_2	Ar	CO_2	$Ca(OH)_2$	$CaCO_3$	CaO	H_2O	
1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	77.13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1388.39	1388.39
2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.18	0.00	0.18
3	0.00	0.00	0.00	0.00	25.00	0.00	0.00	54379.78	0.00	0.00	0.00	0.00	1850.00	0.00	0.00	978835.98	980685.98
4	44363.64	11903.41	528.41	22.73	0.00	0.00	0.00	0.00	1242181.82	380909.09	21136.36	1000.00	0.00	0.00	0.00	0.00	1645227.27
5	0.00	0.00	0.00	0.00	2.27	22.73	0.00	54402.50	0.00	0.00	0.00	0.00	168.18	2272.73	0.00	979245.07	981685.98
6	44363.64	11903.41	528.41	0.00	0.00	0.00	0.00	0.00	1242181.82	380909.09	21136.36	0.00	0.00	0.00	0.00	0.00	1644227.27
7	0.00	0.00	0.00	0.00	2.27	0.00	0.00	54348.10	0.00	0.00	0.00	0.00	168.01	0.00	0.00	978265.82	978433.84
8	0.00	0.00	0.00	0.00	0.00	22.73	0.00	54.40	0.00	0.00	0.00	0.00	0.17	2272.73	0.00	979.25	3252.14
9	0.00	0.00	0.00	0.00	0.00	0.00	22.73	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1272.73	0.00	1272.73
10	0.00	0.00	0.00	22.73	0.00	0.00	0.00	54.40	0.00	0.00	0.00	1000.00	0.00	0.00	0.00	979.25	1979.25
11	0.00	0.00	0.00	22.73	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1000.00	0.00	0.00	0.00	0.00	1000.00
12	0.00	0.00	0.00	0.00	2.27	0.00	0.00	54325.37	0.00	0.00	0.00	0.00	167.94	0.00	0.00	977856.73	978024.68
13	0.00	0.00	0.00	0.00	25.00	0.00	0.00	54302.65	0.00	0.00	0.00	0.00	1849.76	0.00	0.00	977447.64	979297.40
14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	22.73	0.00	0.00	0.00	0.00	0.07	0.00	0.00	409.09	409.16
15	0.00	0.00	0.00	0.00	0.00	0.00	0.00	54.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00	979.25	979.25
16	Boundary flow with impacts assessed through Ecoinvent data set: 'lime production, hydraulic - RoW - lime, hydraulic' & 'tap water production, underground water without treatment - RoW - tap water'																N/A
17	Boundary flow with impacts assessed through Ecoinvent data set: 'natural gas production - US - natural gas, high pressure' & stochiometric evaluation of emissions (CH4 & CO2)																

Lifecycle Assessment (LCA) Data:

Indicator	Value	Unit
Global Warming Potential (GWP)	-193.430083	kg CO_2-eq. / FU
Ozone Depletion	0.000004	kg CFC-11-eq. / FU
Metal Resource Depletion	1.657600	kg Cu-eq. / FU
Freshwater Eutrophication Potential	0.055347	kg P-eq. / FU
Marine Eutrophication Potential	0.077107	kg N-eq. / FU
Acidification Potential	0.362655	kg SO_2-eq. / FU
Water Use	1.633849	m^3 / FU

Technoeconomic Assessment (TEA) Data:

Variable	Value	Unit
$CaCO_3$ calcination	4072.73	MJ / FU
Water evaporation during calcination	2459.86	MJ / FU
CO_2 compression	396	MJ / FU
Total:	6928.59	MJ / FU

Variable	Value	Unit
Energy Input	6928.59	MJ / FU
Theoretical Energy Requirement	6275.331	MJ / FU
Achieved Energy Efficiency	0.9057	Decimal
Overall Relative Energy Efficiency:	0.9057	Decimal

Variable	Value	Unit
Mass Fed (Total)	1646615.85	kg / FU
Mass of Product	1000	kg / FU
Theoretical Maximum Mass Efficiency	1	Decimal
Achieved Mass Efficiency	1	Decimal
Overall Relative Mass Efficiency:	1	Decimal

Flow	Price Data / FU	Data Currency	Year	Price 2022£ / FU:	Quantity Req. (FU):	Total Value:	Unit
Liquified CO_2 from $Ca(OH)_2$ based DAC	1000	USD	2011	812.42	1	812.42	£ / FU
					Total:	812.42	£ / FU

Social Impact Assessment (SIA) Data:

Indicator	Sub-Indicator(s)	Sub-Indicator Value(s)	Final Aggregated Indicator Score
Occupational Health and Safety (OSH)	Accidents causing >4 days' absence	0.929700422	0.704720447
	Work-related disease	0.613791293	
	Work-related mortality	0.640351009	
Child Labour	Non-hazardous	0.90376569	0.899666513
	Hazardous		
	Vulnerability	0.895567336	
Forced Labour	Prevalence	0.980493285	0.938030311
	Vulnerability	0.895567336	
Access to Electricity	Energy imports, net (% of energy use)	0.385998306	0.288767776
	Fossil fuel energy consumption (% of total)	0.211374489	
	Electric power consumption (kWh per capita)	0.127761537	
	Renewable energy consumption (% of total final energy consumption)	0.1717	
Access to Water	Freshwater withdrawal as % of total	0.841279221	0.75313001
	Water Stress	0.664980811	
Land Use Change	-	0.245190502	0.245190502
Utilisation of Hazardous Materials	Deaths caused by dangerous substances per 10,000 workers	0.613788717	0.613788717

Aggregated Final Objective Indicator Scores:

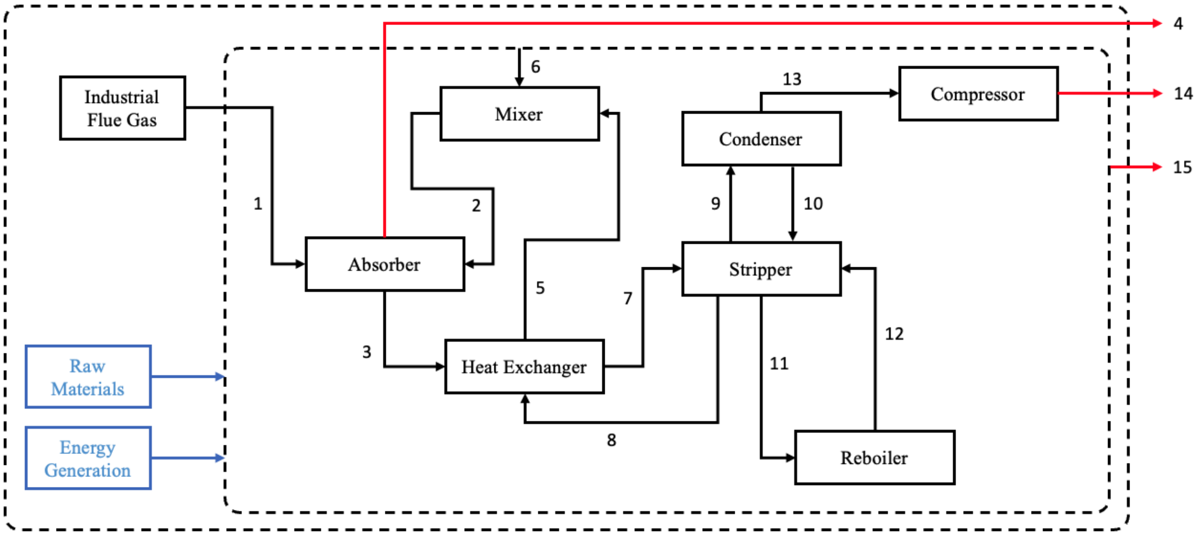
Assessment Strand:	Indicator:	Value:	Units:
LCA	Global Warming Potential (GWP)	-193.430083	kg CO_2-eq. / FU
	Ozone Depletion	0.000004	kg CFC-11-eq. / FU
	Metal Resource Depletion	1.657600	kg Cu-eq. / FU
	Freshwater Eutrophication Potential	0.055347	kg P-eq. / FU
	Marine Eutrophication Potential	0.077107	kg N-eq. / FU
	Acidification Potential	0.362655	kg SO_2-eq. / FU
	Water Use	1.633849	m^3 / FU
TEA	Energy Demand	6928.59	MJ / FU
	Energy Efficiency (%)	0.9057	%
	Mass Efficiency (%)	1	%
	Est. Purchase Price (2022 £)	812.42	2022 £ / FU
SIA	Occupational Health and Safety (OSH)	0.704720447	-
	Child Labour	0.899666513	-
	Forced Labour	0.938030311	-
	Access to Electricity	0.288767776	-
	Access to Water	0.753130016	-
	Land Use Change	0.245190502	-
	Utilisation of Hazardous Materials	0.613788717	-

Spoke Data Sheet (I.D. 3.4)
(CO_2 from Industrial Point Sources)

Inventory Overview:

Quantity:	Character:
Input or Output?	Input
Reference Flow	1 tonne CO_2 via MEA Absorption
Scope	Cradle-to-Gate
Geographic Region	India
Timeframe	2022

System Boundary Block Flow Diagram (BFD):



Spoke Description:

Dataset represents the production of 1 tonne of liquefied CO_2 from industrial flue gas. A portion of the inventory in this dataset is adapted from Ecoinvent v3.8 based on a Swiss study about different cooling mediums. The carbon dioxide is assumed to be obtained free of environmental burdens, as it is considered to be a waste gas of other production processes. The water exchanges are approximated based on data from a large chemical factory.

Standard MEA-based solvents are used for the capture process. In this, an absorber is used to facilitate uptake CO_2 absorption into the solvent (MEA), forming a stable compound. The CO2-rich solvent from the absorber is then passed to a stripping column; heat is applied to the MEA solvent, causing the desorption of CO_2 from the solvent, regenerating it. A highly concentrated CO_2 stream exits the top of the stripper in the gaseous phase prior to liquification and compression in the condenser and compressors. The regenerated solvent, having released it's CO_2, is recycled back to the absorber to continue the capture process. However, due to MEA slip losses a small top-up quantity may be required.

Energy demands from the process are met with a combination of natural gas and non-natural gas (waste process heat or district heating) sources. MEA is assumed to have been produced from ethylene oxide and ammonia with a process yield of 95%.

Boundary Flows:

Classification:	Type:	Description:	Notation:
Input(s)	Raw material extraction / production	Ecoinvent is used to evaluate the impact of feedstock extraction from the environment and any subsequent transforming activities (e.g. MEA production)	N/A
	Industrial flue gas	Average emissions of industrial plants suitable for point source capture.	1
Output(s)	Stream 4	Cleaned flue gas	3
	Stream 14	Liquified CO_2 product	14
	Stream 15	Emissions associated with the MEA based CO_2 capture system (construction, energy and direct emissions)	15

Process Units Included:

Classification:	Type:	Description:
Primary	Absorber	Absorption of CO_2 from industrial flue gas into MEA solvent at 40ºC.
	Mixer	Mixing of CO2 recycle stream with required top-up quantities.
	Heat Exchanger	Recovery of heat from CO_2 lean MEA stripper outlet to heat CO_2 rich MEA for feed to stripper.
	Stripper	Removal of absorbed CO_2 from MEA stream at 120ºC and 2-4 atm.
	Condenser	Removal of water vapour from the stripper overhead gas outlet.
	Reboiler	Reboiling of water for steam used on stripping column.

Assumptions:

Aspect:	Assumption(s):
System Boundary	• The flue gas used is assumed to have been cleaned to conform with release requirements (desulphurisation, etc. completed before being fed to capture system). • Energy provision impacts from existing plants are assumed to be broadly reflective (Ecoinvent, 2021). • Cost of plant operation is obtained from literature based on standard MEA solution and a 555 Mwe NGCC power plant (Putta, et al., 2022). • Flue gas from industrial processes are available for CO_2 capture at zero cost. • 2022 USD to GBP conversion rate is given as 0.7501 as the year's average (Exchange Rates UK, 2024).
Mass balance	• MEA's CO2 absorption capacity in operational plants is 0.53 mol CO_2 /mol MEA (Lv, et al., 2015), removing the requirement to model the absorption mechanism. • BFD adapted from base case MEA capture process presented by Oko, et al. (Oko, et al., 2017) • Industrial flue gas composition is assumed to be comparable to that of natural gas-fired powerplants, detailed by (Song, et al., 2004) • 99.5% CO_2 recovery (Ecoinvent, 2021). • Only CO_2 removed from the flue gas stream. • MEA slip in absorber identified through primary data as 13 kg MEA / tonne CO_2 captured (Ecoinvent, 2021). • Water top-up provided with MEA feed stream. • Recovered CO2 constitutes a negative emission for carbon accounting within the spoke set. • MEA not vaporised in the stripper (120ºC operating temperature) due to the high boiling point of 170ºC (National Institute of Standards and Technology, 2023).
Energy balance	• Energy requirements for CO_2 capture are taken as an average of energy intensity across a range of waste gasses (Ecoinvent, 2021) • Energy provided as heat from a mixture of natural gas and non-natural gas sources (Ecoinvent, 2021) • Energy efficiency of heat provision is assumed to be equal to that of typical industrial furnace and heat exchanger arrangements (90%) (Mickey, 2017)
Waste handling	• Gaseous emissions are directly vented. • Liquid effluents released to waterways
Transportation	• Not included
Miscellaneous	• None

Stream Table:

Stream	Species (kmol/hr)						Species (kg/hr)						Total
	CO2	MEA	H2O	O2	N2	CH4	CO2	MEA	H2O	O2	N2	CH4	
1	22.84090909	0	48.21969697	7.613636364	175.1136364	0.625	1005	0	867.9545455	243.6363636	4903.181818	10	7029.773
2	0	42.8816467	77.77272727	0	0	0	0	1929.674099	1399.909091	0	0	0	3329.583
3	22.72727273	42.5930103	48.21969697	0	0	0	1000	1916.685463	867.9545455	0	0	0	3784.640
4	0.113636364	0.28863636	77.77272727	7.613636364	175.1136364	0.625	5.000	12.98863636	1399.909091	243.6363636	4903.181818	10	6574.716
5	0	42.5930103	48.21969697	0	0	0	0	1916.685463	867.9545455	0	0	0	2784.640
6	0	0.28863636	29.5530303	0	0	0	0	12.98863636	531.9545455	0	0	0	544.943
7	22.72727273	42.5930103	48.21969697	0	0	0	1000	1916.685463	867.9545455	0	0	0	3784.640
8	0	42.5930103	48.21969697	0	0	0	0	1916.685463	867.9545455	0	0	0	2784.640
9	22.72727273	0	48.21969697	0	0	0	1000	0	867.9545455	0	0	0	1867.955
10	0	0	48.21969697	0	0	0	0	0	867.9545455	0	0	0	867.955
11	0	0	48.21969697	0	0	0	0	0	867.9545455	0	0	0	867.955
12	0	0	48.21969697	0	0	0	0	0	867.9545455	0	0	0	867.955
13	22.72727273	0	0	0	0	0	1000	0	0	0	0	0	1000.000
14	22.72727273	0	0	0	0	0	1000	0	0	0	0	0	
15	Boundary flow with impacts assessed through Ecoinvent data set: 'carbon dioxide production, liquid - RoW - carbon dioxide, liquid' Note: This												N/A

Lifecycle Assessment (LCA) Data:

Indicator	Value	Unit
Global Warming Potential (GWP)	-185.610000	kg CO_2-eq. / FU
Ozone Depletion	0.000023	kg CFC-11-eq. / FU
Mineral Resource Depletion	56.756000	kg Cu-eq. / FU
Freshwater Eutrophication Potential	0.214090	kg P-eq. / FU
Marine Eutrophication Potential	0.623700	kg N-eq. / FU
Acidification Potential	2.310900	kg SO_2-eq. / FU
Water Use	3.736700	m^3 / FU

Technoeconomic Assessment (TEA) Data:

Variable	Value	Unit
MEA based CO_2 Capture	3,377	MJ / FU
Total:	3377	MJ / FU

Variable	Value	Unit
Energy Input	3,377	MJ / FU
Theoretical Energy Requirement	3039.3	MJ / FU
Achieved Energy Efficiency	0.9	Decimal
Overall Relative Energy Efficiency:	0.9	Decimal

Variable	Value	Unit
Mass Fed (Total)	7574	kg / FU
Mass of Product	1000	kg / FU
Theoretical Maximum Mass Efficiency	0.1326	Decimal
Achieved Mass Efficiency	0.1320	Decimal
Overall Relative Mass Efficiency:	0.9954	Decimal

Flow	Price Data / FU	Data Currency	Year	Price 2022£ / FU:	Quantity Req. (FU):	Total Value:	Unit
Liquified CO_2	47	USD	2022	35.25	1	35.25	£ / FU
					Total:	35.25	£ / FU

Social Impact Assessment (SIA) Data:

Indicator	Sub-Indicator(s)	Sub-Indicator Value(s)	Final Aggregated Indicator Score
Occupational Health and Safety (OSH)	Accidents causing >4 days' absence	0.689048485	0.611831817
	Work-related disease	0.591438057	
	Work-related mortality	0.582529508	
Child Labour	Non-hazardous	0.769874477	0.607493035
	Hazardous		
	Vulnerability	0.445111594	
Forced Labour	Prevalence	0.941653378	0.693382486
	Vulnerability	0.445111594	
Access to Electricity	Energy imports, net (% of energy use)	0.656944762	0.476854934
	Fossil fuel energy consumption (% of total)	0.264230209	
	Electric power consumption (kWh per capita)	0.01384559	
	Renewable energy consumption (% of total final energy consumption)	0.3293	
Access to Water	Freshwater withdrawal as % of total	0.66115443	0.498116751
	Water Stress	0.335079072	
Land Use Change	-	0.194659486	0.194659486
Utilisation of Hazardous Materials	Deaths caused by dangerous substances per 10,000 workers	0.591436178	0.591436178

Aggregated Final Objective Indicator Scores:

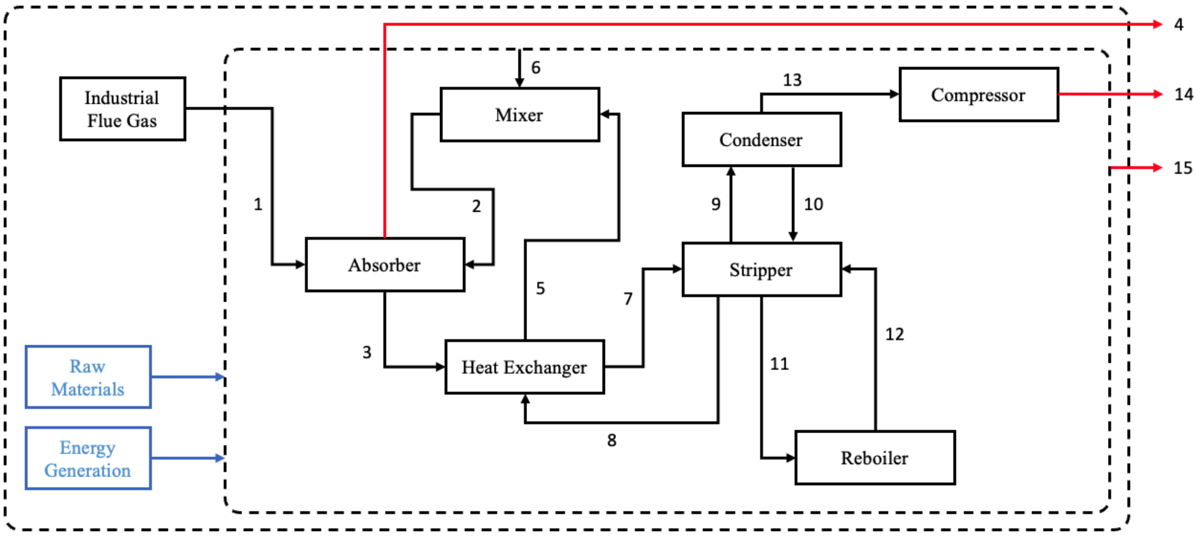
Assessment Strand:	Indicator:	Value:	Units:
LCA	Global Warming Potential (GWP)	-185.610000	kg CO_2-eq. / FU
	Ozone Depletion	0.000023	kg CFC-11-eq. / FU
	Metal Resource Depletion	56.756000	kg Cu-eq. / FU
	Freshwater Eutrophication Potential	0.214090	kg P-eq. / FU
	Marine Eutrophication Potential	0.623700	kg N-eq. / FU
	Acidification Potential	2.310900	kg SO_2-eq. / FU
	Water Use	3.736700	m^3 / FU
TEA	Energy Demand	3377	MJ / FU
	Energy Efficiency (%)	0.9	%
	Mass Efficiency (%)	0.9954	%
	Est. Purchase Price (2022 £)	35.25	2022 £ / FU
SIA	Occupational Health and Safety (OSH)	0.611831817	-
	Child Labour	0.607493035	-
	Forced Labour	0.693382486	-
	Access to Electricity	0.476854934	-
	Access to Water	0.498116751	-
	Land Use Change	0.194659486	-
	Utilisation of Hazardous Materials	0.591436178	-

Spoke Data Sheet (I.D. 3.6)
(CO_2 from Industrial Point Sources)

Inventory Overview:

Quantity:	Character:
Input or Output?	Input
Reference Flow	1 tonne CO_2 via MEA Absorption
Scope	Cradle-to-Gate
Geographic Region	India
Timeframe	2022

System Boundary Block Flow Diagram (BFD):



Spoke Description:

Dataset represents the production of 1 tonne of liquefied CO_2 from industrial flue gas. A portion of the inventory in this dataset is adapted from Ecoinvent v3.8 based on a Swiss study about different cooling mediums. The carbon dioxide is assumed to be obtained free of environmental burdens, as it is considered to be a waste gas of other production processes. The water exchanges are approximated based on data from a large chemical factory.

Standard MEA-based solvents are used for the capture process. In this, an absorber is used to facilitate uptake CO_2 absorption into the solvent (MEA), forming a stable compound. The CO2-rich solvent from the absorber is then passed to a stripping column; heat is applied to the MEA solvent, causing the desorption of CO_2 from the solvent, regenerating it. A highly concentrated CO_2 stream exits the top of the stripper in the gaseous phase prior to liquification and compression in the condenser and compressors. The regenerated solvent, having released it's CO_2, is recycled back to the absorber to continue the capture process. However, due to MEA slip losses a small top-up quantity may be required.

Energy demands from the process are met with a combination of natural gas and non-natural gas (waste process heat or district heating) sources. MEA is assumed to have been produced from ethylene oxide and ammonia with a process yield of 95%.

Boundary Flows:

Classification:	Type:	Description:	Notation:
Input(s)	Raw material extraction / production	Ecoinvent is used to evaluate the impact of feedstock extraction from the environment and any subsequent transforming activities (e.g. MEA production)	N/A
	Industrial flue gas	Average emissions of industrial plants suitable for point source capture.	1
Output(s)	Stream 4	Cleaned flue gas	3
	Stream 14	Liquified CO_2 product	14
	Stream 15	Emissions associated with the MEA based CO_2 capture system (construction, energy and direct emissions)	15

Process Units Included:

Classification:	Type:	Description:
Primary	Absorber	Absorption of CO_2 from industrial flue gas into MEA solvent at 40ºC.
	Mixer	Mixing of CO2 recycle stream with required top-up quantities.
	Heat Exchanger	Recovery of heat from CO_2 lean MEA stripper outlet to heat CO_2 rich MEA for feed to stripper.
	Stripper	Removal of absorbed CO_2 from MEA stream at 120ºC and 2-4 atm.
	Condenser	Removal of water vapour from the stripper overhead gas outlet.
	Reboiler	Reboiling of water for steam used on stripping column.

Assumptions:

Aspect:	Assumption(s):
System Boundary	• The flue gas used is assumed to have been cleaned to conform with release requirements (desulphurisation, etc. completed before being fed to capture system). • Energy provision impacts from existing plants are assumed to be broadly reflective (Ecoinvent, 2021). • Cost of plant operation is obtained from literature based on standard MEA solution and a 555 Mwe NGCC power plant (Putta, et al., 2022). • Flue gas from industrial processes is available for CO_2 capture at zero cost. • 2022 USD to GBP conversion rate is given as 0.7501 as the year's average (Exchange Rates UK, 2024).
Mass balance	• MEA's CO2 absorption capacity in operational plants is 0.53 mol CO_2 /mol MEA (Lv, et al., 2015), removing the requirement to model the absorption mechanism. • BFD adapted from base case MEA capture process presented by Oko, et al. (Oko, et al., 2017) • Industrial flue gas composition is assumed to be comparable to that of natural gas-fired powerplants, detailed by (Song, et al., 2004) • 99.5% CO_2 recovery (Ecoinvent, 2021). • Only CO_2 removed from the flue gas stream. • MEA slip in absorber identified through primary data as 13 kg MEA / tonne CO_2 captured (Ecoinvent, 2021). • Water top-up provided with MEA feed stream. • Recovered CO2 constitutes a negative emission for carbon accounting within the spoke set. • MEA not vaporised in the stripper (120ºC operating temperature) due to the high boiling point of 170ºC (National Institute of Standards and Technology, 2023).
Energy balance	• Energy requirements for CO_2 capture are taken as an average of energy intensity across a range of waste gasses (Ecoinvent, 2021) • Energy provided as heat from a mixture of natural gas and non-natural gas sources (Ecoinvent, 2021) • Energy efficiency of heat provision is assumed to be equal to that of typical industrial furnace and heat exchanger arrangements (90%) (Mickey, 2017)
Waste handling	• Gaseous emissions are directly vented. • Liquid effluents released to waterways
Transportation	• Not included
Miscellaneous	• None

Stream Table:

Stream	Species (kmol/hr)						Species (kg/hr)						Total
	CO_2	MEA	H_2O	O_2	N_2	CH_4	CO_2	MEA	H_2O	O_2	N_2	CH_4	
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2	0	42.8816467	77.77272727	0	0	0	0	1929.674099	1399.909091	0	0	0	3329.583
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14	22.72727273	0	0	0	0	0	1000	0	0	0	0	0	
15	Boundary flow with impacts assessed through Ecoinvent data set: 'carbon dioxide production, liquid - RoW - carbon dioxide, liquid' Note: This												N/A

Lifecycle Assessment (LCA) Data:

Indicator	Value	Unit
Global Warming Potential (GWP)	-185.610000	kg CO_2-eq. / FU
Ozone Depletion	0.000023	kg CFC-11-eq. / FU
Mineral Resource Depletion	56.756000	kg Cu-eq. / FU
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Marine Eutrophication Potential	0.623700	kg N-eq. / FU
Acidification Potential	2.310900	kg SO_2-eq. / FU
Water Use	3.736700	m^3 / FU

Technoeconomic Assessment (TEA) Data:

Variable	Value	Unit
MEA based CO_2 Capture	3,377	MJ / FU
Total:	3377	MJ / FU

Variable	Value	Unit
Energy Input	3,377	MJ / FU
Theoretical Energy Requirement	3039.3	MJ / FU
Achieved Energy Efficiency	0.9	Decimal
Overall Relative Energy Efficiency:	0.9	Decimal

Variable	Value	Unit
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Mass of Product	1000	kg / FU
Theoretical Maximum Mass Efficiency	0.1326	Decimal
Achieved Mass Efficiency	0.1320	Decimal
Overall Relative Mass Efficiency:	0.9954	Decimal

Flow	Price Data / FU	Data Currency	Year	Price 2022£ / FU:	Quantity Req. (FU):	Total Value:	Unit
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	Work-related disease	0.591438057	
	Work-related mortality	0.582529508	
Child Labour	Non-hazardous	0.769874477	0.607493035
	Hazardous		
	Vulnerability	0.445111594	
Forced Labour	Prevalence	0.941653378	0.693382486
	Vulnerability	0.445111594	
Access to Electricity	Energy imports, net (% of energy use)	0.656944762	0.476854934
	Fossil fuel energy consumption (% of total)	0.264230209	
	Electric power consumption (kWh per capita)	0.01384559	
	Renewable energy consumption (% of total final energy consumption)	0.3293	
Access to Water	Freshwater withdrawal as % of total	0.66115443	0.498116751
	Water Stress	0.335079072	
Land Use Change	-	0.194659486	0.194659486
Utilisation of Hazardous Materials	Deaths caused by dangerous substances per 10,000 workers	0.591436178	0.591436178

Aggregated Final Objective Indicator Scores:

Assessment Strand:	Indicator:	Value:	Units:
LCA	Global Warming Potential (GWP)	-185.610000	kg CO_2-eq. / FU
	Ozone Depletion	0.000023	kg CFC-11-eq. / FU
	Metal Resource Depletion	56.756000	kg Cu-eq. / FU
	Freshwater Eutrophication Potential	0.214090	kg P-eq. / FU
	Marine Eutrophication Potential	0.623700	kg N-eq. / FU
	Acidification Potential	2.310900	kg SO_2-eq. / FU
	Water Use	3.736700	m^3 / FU
TEA	Energy Demand	3377	MJ / FU
	Energy Efficiency (%)	0.9	%
	Mass Efficiency (%)	0.9954	%
	Est. Purchase Price (2022 £)	35.25	2022 £ / FU
SIA	Occupational Health and Safety (OSH)	0.611831817	-
	Child Labour	0.607493035	-
	Forced Labour	0.693382486	-
	Access to Electricity	0.476854934	-
	Access to Water	0.498116751	-
	Land Use Change	0.194659486	-
	Utilisation of Hazardous Materials	0.591436178	-

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