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WP5 Joint integration into an LCSA framework

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EXECUTIVE SUMMARY

This document presents the harmonised Life Cycle Sustainability Assessment (LCSA) guidelines developed within the SH2E project for fuel cells and hydrogen (FCH) systems. Thus, this deliverable provides a unified framework that integrates the separate guidelines for FCH-specific Life Cycle Assessment (LCA), Life Cycle Costing (LCC), and Social Life Cycle Assessment (SLCA). In order to attain this harmonisation, the three individual deliverables previously developed in SH2E were thoroughly analysed identifying shared aspects, areas of divergence requiring harmonisation, and areas where some degree of divergence could be preserved, acknowledging the distinct requirements of each sustainability dimension. Additionally, improvement recommendations are provided for non-common elements, and novel topics that enrich the harmonised LCSA framework are addressed. The FCH-LCSA guidelines presented herein offer a coherent, transparent, and methodologically rigorous framework for evaluating the sustainability of FCH systems throughout their life cycle. By aligning and harmonising the LCA, LCC and SLCA methodologies, this framework ensures a comprehensive understanding of the potential environmental, economic and social impacts associated with FCH systems. These guidelines are expected to serve as a valuable support for practitioners and stakeholders to make informed and sustainability-oriented decisions concerning FCH systems.

This deliverable includes illustrative examples of partial LCSA applications, aimed at facilitating the understanding of the SH2E LCSA guidelines. On the other hand, full case studies are provided in SH2E D6.3.

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KEY TERMS

Term	Definition
Allocation	Partitioning the inputs/outputs, considering the different functions and the relationship (preferentially physical relationship) among these
Biogenic carbon	CO_2 uptake through photosynthesis and carbon emissions (CO_2, CO and CH_4) from transformation or degradation of biomass (e.g. due to combustion, landfilling…)
Capital goods	Components such as machinery used in production processes, buildings, office equipment, transport vehicles, and transportation infrastructure
Characterisation	Calculation of category indicator results using characterisation factors for every relevant flow, according to the analysed impact category
Characterisation factor	Factor derived from a characterisation model and applied to convert an assigned life cycle inventory analysis result to the common unit of the category indicator
Cradle-to-Gate	Assessment including all stages from resource extraction to the factory gate
Cradle-to-Grave	Assessment including all stages from resource extraction to the use and disposal phase
Data	Collection of facts or organised information, usually the results of observation, experience, or experiment, or a set of premises from which conclusions may be drawn
Data quality	Characteristics of data that relate to their ability to satisfy stated requirements
Elementary flow	Material or energy entering the system being studied that has been drawn from the environment without previous human transformation, or material or energy leaving the system being studied that is released into the environment without subsequent human transformation
Functional unit	Quantitative representation of the function of the system, which serves as reference for all the flows involved in the assessed system
Hydrogen as a by-product	Hydrogen produced by a system for which hydrogen production is not the main purpose of the process
Hydrogen as a co-product	Hydrogen produced by a system in which hydrogen and other products are key valuable outputs
Hydrogen as the main product	Hydrogen produced by a system that has as the primary goal its production
Impact category	Class representing sustainability issues of concern to which life cycle inventory analysis results may be assigned
Impact category indicator	Quantifiable representation of an impact category
Life cycle sustainability assessment (LCSA)	Methodology to quantitatively assess the potential sustainability impacts of product systems from a holistic perspective
Life cycle sustainability impact assessment	Third phase of the LCSA framework, which aims to evaluate the potential sustainability impacts in the life cycle under study
Life cycle sustainability inventory	It is the result of the second phase of the LCSA framework; it contains information regarding all input and output flows referring to the system boundaries

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Multi-functional system/process	System/process that originates more than one functional flow
Normalisation	It is the process of adjusting disparate criteria or attributes to a common scale for fair and accurate comparison. This technique aims to standardise diverse criteria that may have different units, ranges, or magnitudes into a uniform scale, often between 0 and 1 or another predefined range.
Primary data (raw data)	Data that are collected directly related to their object of study (from meter readings, purchase records, utility bills, engineering models, direct monitoring, etc.)
Secondary data	Data collected by someone else earlier (average industry data, literature data, etc.)
Subdivision	Division of the unit process in different sub-processes
System boundaries	Set of criteria that specify which processes are included in the product system and determine which unit processes shall be included in the LCSA
System expansion	Inclusion of additional functions for products that are not the quantitative reference of the process, allowing to expand the product system
Unit process	Smallest element considered in the life cycle inventory analysis for which input and output data are quantified
Weighting	It is the assignment of relative importance or significance to various indicators/criteria. It involves quantifying the influence or priority of each criterion in relation to others to reflect their impact on the final decision outcome.

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ACRONYMS

AEL	Alkaline Electrolyser
AFC	Alkaline Fuel Cell
CAPEX	Capital Expenditure
CCS	Carbon Capture and Storage
CCU	Carbon Capture and Utilisation
CRM	Critical Raw Material
DAC	Direct Air Capture
EF	Environmental Footprint
EoL	End-of-Life
FCEV	Fuel Cell Electric Vehicle
FCH	Fuel Cells and Hydrogen
FU	Functional Unit
HT-Co-EC	High-Temperature Co-Electrolysis
IAM	Integrated Assessment Model
ILCD	International Reference Life Cycle Data System
LCA	Life Cycle Assessment
LCIA	Life Cycle Impact Assessment
LCC	Life Cycle Costing
LCI	Life Cycle Inventory
LCoH	Levelised Cost of Hydrogen
LCSA	Life Cycle Sustainability Assessment
OPEX	Operational Expenditure
PAFC	Phosphoric Acid Fuel Cell
PEMWE	Proton-Exchange Membrane Electrolyser
PEMFC	Proton-Exchange Membrane Fuel Cell
PSILCA	Product Social Impact Life Cycle Assessment
SLCA	Social Life Cycle Assessment
SMR	Steam Methane Reforming
SOE	Solid Oxide Electrolyser
SOFC	Solid Oxide Fuel Cell
TRL	Technology Readiness Level

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GENERAL INFORMATION

Hydrogen production and use solutions are expected to play a crucial role in the transition to a global sustainable energy system. This document provides methodological guidance on how to perform a Life Cycle Sustainability Assessment (LCSA) of fuel cells and hydrogen (FCH) systems to facilitate informed decision-making, promote sustainability, and ensure consistency and harmonisation in the assessment process. This document is an extension of previous deliverables within the SH2E project. It complements and extends the insights from the separate guidelines for FCH-LCA (D2.2) (Bargiacchi et al., 2022), FCH-LCC (D4.1) (Wulf et al., 2022a) and FCH-SLCA (D4.2) (Iribarren et al., 2023), taking into account the lessons learned in previous tasks of the SH2E project. This document embraces hydrogen production, hydrogen use and hydrogen production & use systems. It promotes a harmonised and consistent evaluation of the potential life-cycle sustainability impacts of FCH products through robust, well-defined methods to effectively support case-specific accounting and decision-making processes, also providing examples for practical application.

The present guidelines are targeted at any practitioner conducting LCSA studies of FCH systems (hydrogen production, hydrogen use, or hydrogen production & use). The practitioner is guided on how to deal with the methodological aspects of an LCSA (functional unit, system boundaries, etc.) and specific topics relevant to FCH systems (e.g. supply chain segmentation or data sources). This document aims to provide a robust foundation for conducting LCSA studies in the context of FCH systems, ultimately contributing to the sustainable development and use of hydrogen-related technologies.

How to use this document

The document provides guidance on how to conduct an LCSA of FCH systems. The provisions, recommendations and supplementary information are clearly identified in the document according to the following colour code:

In the green boxes, requirements are presented.

In the light blue boxes, recommendations are presented.

In the yellow boxes, supplementary information is reported.

Each of these boxes may include illustrative examples (grey boxes along the document) aimed at facilitating the practical application of the LCSA. Those examples have been either developed explicitly within the context of this deliverable or retrieved from external sources. Regarding the latter, it is important to remark that those examples might not involve entirely SH2E-compliant LCSA studies (which would require hydrogen-related studies addressing the three dimensions of sustainability and strictly conducted according to the guidelines delivered in this project). This is mainly due to the current scarce literature on the matter. However, they were considered suitable references to illustrate how each of the topics could be addressed.

The different topics in the guidelines have also been evaluated in terms of their "method readiness level", i.e., a score identifying the level of development of the addressed topic under the following scheme:

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Method readiness level	Meaning	Symbol
5	Method already implemented in LCSA tools	●●●●●
4	Data available for established method	●●●●○
3	Established method	●●●○○
2	Ongoing discussions on the method	●●○○○
1	First ideas on the method	●○○○○

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GUIDANCE ON PERFORMING LIFE CYCLE SUSTAINABILITY ASSESSMENT OF FCH SYSTEMS

1. Introduction

Within the SH2E project, the methodological framework proposed for Life Cycle Sustainability Assessment (LCSA) follows the approach recommended by Valdivia et al. (2011). LCSA, as embraced in this framework, represents a harmonised combination of three key life-cycle techniques: environmental Life Cycle Assessment (LCA) (International Organization for Standardization, 2006a, 2006b), Life Cycle Costing (LCC) (Swarr et al., 2011), and Social Life Cycle Assessment (SLCA) (UNEP, 2020). It is important to note that the overall outcomes of LCSA should be interpreted as a synergistic combination of the results derived from each individual technique.

LCSA is an iterative process composed of **four interrelated phases** (European Commission, 2010; Valdivia et al., 2011):

- **Goal and scope definition***:* This phase involves defining the overarching purpose of the LCSA study, including the intended applications and the decision-making context. The scope sets the boundaries of the study, specifying aspects such as the system under analysis, its function and functional unit, the covered life-cycle stages, assumptions, stakeholders, methodological choices, sustainability impacts to be investigated, and the selected impact assessment methods.
- **Life cycle inventory analysis**: This phase entails systematically gathering data flows along the product's supply chain, which are subsequently fed to the environmental, economic, and social impact assessments.
- **Life cycle impact assessment**: During this phase, the inventory data of the LCSA study are evaluated to characterise the life-cycle sustainability performance of the product system. The selection of the assessed categories and indicators depends on a materiality assessment that takes into account stakeholders' perspectives.
- **Interpretation:** The interpretation phase involves the analysis of previous results to identify key contributions and potential areas for improvement. It can also enable technological or scenario benchmarking. This phase may encompass robustness tests, sensitivity analyses, uncertainty analyses, completeness analyses, and consistency checks. Results are recommended to be interpreted in a combined manner, identifying potential trade-offs across sustainability dimensions.

This document incorporates insights gained from the **individual life-cycle guidelines** developed within the SH2E project (Bargiacchi et al., 2022; Wulf et al., 2022a; Iribarren et al., 2023). While other projects such as ORIENTING have proposed LCSA recommendations with generic applicability (Pihkola et al., 2022), the focus of this work was placed on offering practitioners a deeper understanding of the specific aspects in the specific field of **fuel cells and hydrogen (FCH) systems**, going beyond past initiatives (Lozanovski et al., 2011; Massoni et al., 2011). Consequently, the SH2E LCSA guidelines identify and promote good practices for LCSA of FCH systems, providing a valuable framework for practitioners and stakeholders to make informed, sustainability-oriented decisions. Moreover, these guidelines could also be relevant to other systems closely linked to hydrogen ones, as illustrated in **Annex 1**.

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Model asymmetry

It is essential to acknowledge that –throughout the LCSA process– some decisions may prove challenging to harmonise across the three sustainability domains commonly encompassed by LCSA (Valdivia et al. 2011, 2021). This document acknowledges that **model asymmetries** may exist where certain aspects or data may not seamlessly align across all sustainability dimensions within the LCSA framework. These asymmetries are point-by-point acknowledged in these guidelines to provide transparency and guidance to LCSA practitioners (UNEP, 2017). It is imperative for practitioners to be aware of such asymmetries and exercise caution when attempting to integrate data or assessments that may not perfectly align across all dimensions (Costa et al., 2019).

The following sections of this document offer detailed guidelines and recommendations for LCSA of FCH systems, considering both well-established practices and specific considerations in the FCH sector.

2. Goal of the Life Cycle Sustainability Assessment

Motivation

The goal of an LCSA establishes the basis capable of correctly answering the questions posed by/to the practitioner. Hence, it strongly influences the whole setup of an LCSA, comprising **goal and scope, data, and quality assurance**. This especially concerns the application situation since LCSA is envisaged to be a tool of increasing relevance for decision making (UNEP, 2017; Valdivia et al., 2021). Although LCA, LCC and SLCA may have different aims because they are application-dependent, **a common goal and a common scope are strongly recommended** when undertaking a combined LCSA. This alignment ensures that the diverse objectives of these methodologies converge, creating a unified and coherent framework. This unity facilitates a holistic assessment that captures the interaction between environmental, economic and social dimensions. Overall, the motivation behind an LCSA study serves as the driving force that sets its purpose and direction. It aligns the assessment process with the questions and challenges posed by stakeholders, making LCSA a powerful instrument for promoting sustainability and facilitating informed decision-making (Backes and Traverso, 2022).

Description of the topic and key terms

Goal definition is the first step in an LCSA. It defines and explains the purpose of the study by answering three main questions related to: expected use of the LCSA results, application situation, and reasons for carrying out the study. These aspects are strongly linked to each other. All of them have implications in subsequent LCSA aspects (e.g. modelling approach and inventory building) and must be coherent with the practitioner's core question.

Intended application(s)

The **expected use** of the LCSA results could be more than one for a given LCSA study. It seeks to understand how the results will be used and who the primary stakeholders are. This consideration is pivotal, as it ensures that the LCSA is adapted to provide relevant information for decision-making processes. The foreseen applications affect not only the LCSA model construction, but also the modelling perspective. For instance, FCH systems often fall into the prospective / new technology category.

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Application situation and reasons for carrying out the study

The **application situation**, also referred to as decision context, is intimately linked to the intended application(s) since, depending on the expected use of the LCSA results, one modelling approach may be more appropriate than another. Additionally, the application situation may be conditioned by the specific dimension to be evaluated within the LCSA study.

The reasons to carry out an LCSA study answer why the LSCA study is made. It could also be understood as the core question determining the stakeholders involved as well as the model prepared to answer it. Understanding the motivations behind conducting the LCSA is key. It requires a thoughtful examination of why the assessment is being undertaken. This question helps identify the driving forces, sustainability concerns, or specific issues that prompt the study.

Stakeholder perspective

In the pursuit of a harmonised LCSA framework, key topics of the goal and scope definition, such as the system boundaries and the selection of impact categories, play a pivotal role in evaluating the holistic sustainability performance of FCH systems. To ensure robust choices, the incorporation of **stakeholder perspectives** is strongly recommended (cf. Section 3.5). This approach is aligned with the overarching goal of harmonisation and enhances the credibility and applicability of LCSA outcomes.

Box 1 Stakeholder perspective

The stakeholder perspective needs to be stated in the Goal & Scope Definition phase of the LCSA study.

Example: (from reference [Wulf et al., 2023], on hydrogen-based mobility)

"Our previously developed approach for sustainability assessment is used to carry out an indicator-based sustainability assessment of different hydrogen mobility options in Germany. Within the framework of the extended approach, weighting factors for sustainability indicators and dimensions are determined through a stakeholder survey and are used for the aggregation of indicators with the MCDA method Preference Ranking Organization METHod for Enrichment of Evaluations (PROMETHEE)."

Requirements and recommendations

Importantly, when combining the three assessment methodologies (LCA, LCC and SLCA) within an LCSA framework, it is advisable to **ensure alignment** in the questions posed across the sustainability domains. While each methodology may involve different choices and approaches, coherence in the overall goal definition is essential (Valdivia et al., 2011, 2021). Hence, the three aforementioned questions (expected use of the results, application situation, and reasons for the study) should be asked consistently across the environmental, economic and social dimensions as far as possible, reflecting a holistic understanding of sustainability. It is crucial to acknowledge that there may be cases where the individual methodologies within the LCSA are not technically prepared to address some of these questions in a combined framework. In that case, practitioners should be aware of the **limitations and challenges**, and consider alternative approaches or adaptations to ensure as much alignment as possible.

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Box 2 Intended application of the LCSA

The intended application must be considered for LCSAs. The intended application is characterised by the intended modelling perspective and approach. The application situation must be coherent with it, by stating if the LCSA study is to be used for decision support (yes/no) and also stating the scale of the induced changes in the considered system. The alignment of these aspects across all dimensions is essential to ensure that the LCSA is a coherent tool for guiding decision-making processes. In some cases, the individual life-cycle methodologies may have limitations in addressing certain aspects of the intended application. Practitioners should be aware of these limitations and consider alternative approaches or adaptations to ensure alignment to the extent possible.

Example: (from SH2E deliverable D6.3, regarding the prospective LCSA of a high-temperature hydrogen production system)

"Although the progressive implementation of renewable hydrogen pathways is expected to have a large scale-effect, this study places the focus on accounting for potential environmental impacts of the specific hydrogen product, with decision support limited to the specific product (i.e. micro-level decision support)."

In terms of communication strategies, the practitioner should prioritise transparency by explicitly addressing the **limitations of the LCSA study**, including those arising from asymmetry across the three individual life-cycle methodologies (LCA, LCC and SLCA). These limitations can manifest in various ways, including differences in data availability and/or methodological choices across sustainability domains. By acknowledging and transparently communicating these limitations, the practitioner ensures that the study results are appropriately interpreted and used for decision-making processes (Valdivia et al., 2021). This proactive approach helps practitioners to prevent the potential misuse or misrepresentation of LCSA findings to serve specific interests by individuals, companies or public institutions. Moreover, it promotes a more refined understanding of the study's outcomes, encouraging stakeholders to consider the integrated sustainability assessment in a responsible and informed manner, while recognising the inherent challenges posed by model asymmetry.

Box 3 Limitations of the study

The LCSA practitioner has to state clearly the limitations of the study in terms of use (asymmetry of the individual methodologies) and interpretation of the LCSA results. This is even more important when it comes to comparative LCSA studies being disclosed to the public.

Example: (from SH2E deliverable D6.3, regarding the prospective LCSA of a high-temperature hydrogen production system)

"As this study places the focus on estimating and benchmarking the (prospective) life-cycle environmental profile of hydrogen from SOE, it should not be directly used to guide decision-making at meso or macro level. Moreover, this study should be understood as case-specific and not intended to generalise the environmental findings of the study."

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Evaluation: "method readiness level"

- Consideration of the application situation in LCSA ●●●●○

This section is linked to the following sections of the present guidelines:

- 3: Scope of the Life Cycle Sustainability Assessment
- 3.5: Materiality assessment and stakeholder engagement
- 4: Life Cycle Inventory
- 5: Life Cycle Impact Assessment

3. Scope of the Life Cycle Sustainability Assessment

Section 3 addresses key aspects on the scope of the LCSA study, including **modelling approach** (Section 3.1), **functional unit** (Section 3.2), and **system boundaries** (Section 3.3). In defining the LCSA scope, it is essential to consider the challenges posed by assessing environmental, economic and social impacts within a unified framework.

3.1 Modelling approach

The choice of the most suitable **modelling approach** to evaluate the environmental, economic and social impacts of an FCH product system depends on the stage of development of the core technology (technology readiness level [TRL], manufacturing readiness level [MRL], market deployment) and the goal of the study (e.g. decision level). Depending on the goal of the study, consequential or dynamic modelling can be applied to retrospective or prospective inventories. Regarding the choice of the modelling approach, it dictates the need for different foreground and background data sources, which may be retrieved from literature or dedicated databases. This choice also influences the temporal and geographical dimensions of the study, as well as the definition of the functional unit. When the study is intended to inform policy-making, a consequential modelling approach is highly recommended. It is noteworthy that, despite its potential benefits, consequential modelling remains underrepresented not only in the current LCSA literature specific to FCH systems (cf. Section 3.1.2) but also in the broader context (Costa et al., 2019).

Overall, the scope of the LCSA should be approached with a clear understanding of what is to be included, precisely stating the aspects included or excluded for each sustainability domain. Ideally, the modelling approach and system boundaries of an FCH product system should align across dimensions. However, achieving an exact match in all three dimensions (environmental, economic and social) may not always be feasible due to model asymmetry. While striving for coherence across dimensions, different practical considerations such as the use of databases, the availability of tools, and potential future advancements should be taken into account (Pihkola et al., 2022).

By conscientiously addressing the **LCSA scope**, acknowledging **model asymmetry** and providing a **clear statement**, practitioners can ensure the transparency and coherence of the assessment across sustainability dimensions.

3.1.1 Prospectivity

In the context of LCSA, the used approach can significantly vary based on the developmental stage of the technology or system under study. The **conventional** (and widely applied) **retrospective** approach evaluates the sustainability impacts of a product ex-post at a present time, i.e., when a product has already been commercialised and used for a time and data are widely available (van der Giesen et al., 2020). When the core technology is modelled at a future phase, a **prospective approach** needs to be applied. For FCH technologies, the

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retrospective approach has been largely applied. However, many FCH systems are still at early stages of development or market deployment, where a prospective approach becomes recommended (Bargiacchi et al., 2022; Wulf et al., 2022a; Iribarren et al., 2023).

An LCSA is defined **prospective** when the technology studied is at an early phase of development or market deployment, but it is modelled at a future, more developed phase, reflecting its potential sustainability impacts once fully developed and deployed. This definition has been adapted from Arvidsson et al. (2018) and includes most of the FCH systems. A prospective LCSA study is classified as a forward-looking LCSA approach along with other non-excluding approaches such as anticipatory or ex-ante LCSA.

It is crucial to acknowledge that prospectivity is one of the areas where the individual life-cycle methodologies (LCA, LCC and SLCA) may not have the same level of advancement. Consequently, practitioners should exercise caution and transparency when conducting a prospective LCSA study, particularly with regard to SLCA. In SLCA, obtaining reliable data for prospective suppliers and assessing potential future social conditions can be exceptionally challenging (Iribarren et al., 2023). The uncertainty associated with social aspects in a prospective view requires a careful acknowledgment of these limitations by practitioners. While prospectivity offers valuable insights into the future sustainability implications of emerging technologies, it is essential to communicate the inherent uncertainties and constraints associated with this approach.

Box 4 Prospectivity I

To be prospective within the context of these guidelines, an LCSA study must meet the following requisites:

1. The system must be modelled at a future time.
2. The technical/operating parameters and capital goods of the analysed product system must be prospective.

When performing a comparative study, it must be ensured that the FCH technologies under comparison are modelled at the same future time of implementation.

Example: (from SH2E deliverable D6.3, regarding the prospective LCSA of a high-temperature hydrogen production system)

"The system under evaluation was modelled based on the year 2030, when SOE technology is expected to reach full technical maturity. Thus, the SOE part of the system was modelled according to the expected technical key performance indicators (KPIs) for 2030, while the CSP operating parameters, the integrated performance of the CSP-SOE system and the modelling of the reference hydrogen production system through SMR were based on the use of process simulation tools."

Additionally, the following recommendations should be considered:

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Box 5 Prospectivity II

1. The use of relevant prospective background data for processes directly linked to the foreground system (e.g. electricity production) is strongly recommended to the extent possible for each sustainability dimension.
2. It is recommended to state the TRL and/or the MRL of the involved technology to facilitate comparability decisions.
3. Limitations related to prospectivity should be clearly stated for transparency.

Example:

Consult **Annex 2** of this deliverable.

Specific information on scale effects and learning phenomena can be found in the Section 3.1.1 of the SH2E deliverable D2.2 on FCH-LCA guidelines (Bargiacchi et al., 2022).

Evaluation: "method readiness level"

The approach on how to handle prospectivity in LCSA is twofold:

- Through the inventory by using prospective foreground and/or background data ●●○○○
- Through the impact assessment method by using prospective characterisation factors ●○○○○

3.1.2 Consequentiality

The **consequential approach** within LCSA is a methodological perspective that evaluates the sustainability impacts of a product or system by considering the potential changes it induces within the broader socio-economic and environmental context. It is important to note that the consequential approach, while feasible in the three individual methodologies (LCA, LCC and SLCA), has not been equally advanced in each dimension (Costa et al., 2019). Specifically, consequentiality in SLCA may require further development and refinement to achieve a level of sophistication comparable to that in environmental and economic assessments (Sousa-Zomer and Cauchick Miguel, 2018). Nonetheless, this should not discourage its application in the social dimension when affordable.

By recognising the varying levels of advancement in the consequential approach and its feasibility, particularly in SLCA, practitioners can make conscious decisions when selecting the appropriate approach for their specific LCSA study, taking into account the potential for enhancing the state of the art in sustainability assessment.

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Box 6 Consequentiality I

If the LCSA study is aimed at a macro-level decision (e.g. policy-making), a consequential approach has to be followed to the extent possible for each sustainability dimension.

Example: (from reference [Ortigueira et al., 2020], on the consequential LCA of biohydrogen production through dark fermentation)

"The present study explored the use of separately-collected food waste for the fermentative production of H_2-rich biogas to operate a PEMFC […] To make the comparison in terms of direct energy consumption and global warming potential (GWP100 years), a consequential approach was followed, i.e. marginal supply and demand on affected markets was taken into consideration and allocation was avoided by system expansion."

Box 7 Consequentiality II

1. The identified marginal technologies should be clearly stated and reported, including a justification on the choice of the marginal technologies and the procedure followed for that identification.
2. The quantification of the change in marginal technologies should be clearly stated, reported and justified, clearly specifying the procedure followed for that quantification.
3. The quantification of the sustainability impacts of the change should be clearly reported (data sources, procedure, results, etc.).
4. Besides that, the following recommendations apply:
   - Whenever an economic model is applied, the user should give full traceability of the economic models/equations applied and the input data used for the study.
   - A clear statement of the time horizon of the consequences (short, medium, long term) is recommended.
   - Whenever a consequential approach is needed, it is recommended to evaluate results for different models, especially if applied in the context of policy-making.

Further information about consequentiality can be found in the Section 3.1.2 of the SH2E deliverable D2.2 on FCH-LCA guidelines (Bargiacchi et al., 2022).

Evaluation: "method readiness level"

The approach on how to handle consequentiality in LCSA is the following:

- Consideration of the application in LCSA ●○○○○

3.1.3 Spatial scale

Spatial scale plays a crucial role in LCSA by providing valuable insights into the geographic distribution of impacts across the life cycle of a product. While the mandatory requirement for spatial information primarily applies to SLCA, it is strongly recommended to adopt a consistent spatial scale across the three dimensions (LCA, LCC and SLCA) to ensure coherence in the assessment, including the location of each of the unit processes within the system boundaries. In particular, for such regionalisation, **the definition of the location (e.g. country) where the final output is produced arises as a key aspect**, as it determines the

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remaining locations along the corresponding supply chains (cf. Section 3.3). This consistency ensures that the boundaries of the assessed system align across sustainability domains, facilitating a holistic understanding of the interconnected environmental, economic and social dimensions. Further information about spatial scale can be found in the Section 1.5 of the SH2E deliverable 4.2 on FCH-SLCA (Iribarren et al., 2023).

Box 8 Definition of the region where the final output is produced

The LCSA practitioner has to clearly state the location (at least, country specification) of the process that delivers the target function of the system (to which the functional unit is referred).

Example: (from reference [Iribarren et al., 2022], on SLCA and benchmarking of green methanol)

"The green methanol system under study involves methanol production from CO_2 (directly captured from the air) and hydrogen (from wind power electrolysis) at a hypothetical plant in the USA."

Evaluation: "method readiness level"

The approach on how to handle spatial scale in LCSA is the following:

- Consideration of the application in LCSA ●●●●○

This section is linked to the following sections of the present guidelines:

- 3.2: Functional unit
- 3.3: System boundaries
- 4.2: Data sources and availability

3.2 Functional unit

Motivation

The **functional unit** of an LCSA represents the principal function of the system under study, according to the goal and scope of the LCSA. It is linked to a reference flow to which all the inputs and outputs of the system are related. The functional unit is, therefore, a quantitative representation of the main function of the system. In the case of systems providing more than one function (**multi-functional systems**), the practitioner must isolate/choose one of the functions so that LCSA results are related to a single reference flow. Besides, special attention should be paid when carrying out **comparative LCSAs** because the functional unit must represent a common function accomplished at the same level (e.g. hydrogen produced in a specific location with the same degree of purity and with the same final temperature and pressure).

The definition of a **homogeneous functional unit** across the sustainability dimensions of an LCSA study is of paramount importance. Aligning the functional unit with the defined goal and system boundaries of the study ensures the coherent evaluation of environmental, economic and social impacts (Valdivia et al., 2011, 2021). A consistent functional unit allows practitioners to draw meaningful conclusions regarding the trade-offs and synergies between

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sustainability dimensions, facilitating decision-making processes. Therefore, LCSA practitioners must diligently define and apply a functional unit that reflects the primary function of the system, fostering the holistic assessment of the life-cycle sustainability impacts of FCH systems (Bargiacchi et al., 2022; Wulf et al., 2022a; Iribarren et al., 2023).

This section provides guidelines for functional unit definition in LCSA of FCH systems. It considers the previous single-dimension deliverables of the SH2E project: Section 3.2 of the SH2E deliverable D2.2 on FCH-LCA guidelines (Bargiacchi et al., 2022), Section 3.2 of the SH2E deliverable D4.1 on FCH-LCC guidelines (Wulf et al., 2022a), and Section 1.3 of the SH2E deliverable D4.2 on FCH-SLCA guidelines (Iribarren et al., 2023).

Description of the topic

Hydrogen may be involved in a great variety of supply chains (e.g. electricity, fuels, chemicals), and might appear at different stages of the life cycle. It could be used as a fuel itself or used to fulfil another function such as energy storage and chemicals production (e.g. ammonia and methane). This versatile nature allows hydrogen to provide very different functions, which results in the need to define functional units of different sort (Ciroth et al., 2021). Therefore, it is crucial to identify the **main function of the system** and define the functional unit accordingly. In addition, many hydrogen systems are identified as multi-functional ones. For example, the chlor-alkali process could have as main function: chlorine, sodium hydroxide, or hydrogen production, which are corresponding to its three functional flows.

Because of the large heterogeneity observed regarding hydrogen-related systems, this section differentiates between **systems exclusively assessing hydrogen production, and those including its use within the system boundaries.**

Options

Different cases are herein distinguished for functional unit definition:

- **Case 1**: Systems exclusively assessing hydrogen production.
- **Case 2**: Systems including hydrogen use within their system boundaries:
    - 2a. Hydrogen for transportation.
    - 2b. Hydrogen for fuels and chemicals production.
    - 2c. Hydrogen for electricity and/or heat generation.

Requirements and recommendations

General recommendations

Since the concept of functional unit was born in the framework of LCA (International Organization for Standardization, 2006a, 2006b), the general recommendations proposed for functional unit definition build upon the principles outlined in previous individual guidelines (Bargiacchi et al., 2022; Wulf et al., 2022a; Iribarren et al., 2023), while introducing specific considerations tailored to LCSA.

The first step is to identify the function of the system under study. This could be straightforward in the case of systems with a single functional flow or a clear goal. For systems with various functional flows (multi-functional systems), the LCSA practitioner should identify the functional flows as recommended in **Section 3.4 "Multi-functionality"**. Once the functional unit has been selected, the functional flow serving as reference flow of the system must be identified and quantified.

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In addition to these foundational steps, it is imperative to incorporate LCSA-specific considerations into the process of functional unit identification. In this sense, the identification of a functional unit should go beyond single-dimensional considerations. Practitioners must ensure a **homogeneous functional unit** across the three sustainability dimensions (environmental, economic and social). Moreover, the functional unit must be aligned with the overarching goal and scope of the LCSA study (Valdivia et al., 2011, 2021).

Box 9 Identification of functional unit, functional flows and reference flow

1. The function of the system to be assessed must be identified.
2. A homogeneous functional unit aligned with the goal must be established across all three sustainability dimensions within an LCSA study.
3. The functional flows of the system, if more than one, must be identified and reported to clearly state the methodology used for their handling later on (Section 3.4).
4. The reference flow of the system must be indicated and quantified.

In some situations, the identification of the main function of the system may present some difficulties because of the use of hydrogen as an **energy vector** since hydrogen can act as energy transportation or energy storage media. For example, using renewable electricity surplus to produce hydrogen through electrolysis may have as the main goal the production of hydrogen, or just the storage of renewable electricity. The identification of the function of the system is given by a qualitative analysis by the LCSA practitioner, who needs to evaluate whether the goal of the system is to produce hydrogen or to store renewable energy. This discussion is more significant when developing comparative studies because equivalent functions are required. In the case of comparative LCSA, the functional unit must guarantee that the function of the systems is the same. Attention should also be paid to check whether all the systems achieve the minimum level of qualitative requirements set for the function (Bauman and Tillman, 2004). These qualitative considerations are set by the LCSA practitioner depending on the goal of the system (e.g. hydrogen threshold purity for its usage in fuel cells). A clear definition of the qualitative characteristics that the product should attain is key to ensure a fair comparison between different systems. Variations on the reference flow quantity could arise if there are differences in quality or performance among the different systems assessed.

Box 10 Functional unit in comparative LCSA

1. Comparative LCSAs must ensure that the selected functional unit represents the common function of the systems and allows a fair comparison, also considering geographical location of the final output.
2. Qualitative considerations to be achieved by the evaluated systems, which can be made in the form of quantitative thresholds or qualitative statements, must be clearly defined.

Requirements and recommendations for Case 1: Systems exclusively assessing hydrogen production

Regardless of the assessed hydrogen production pathway, a convergence in literature can be observed on the adoption of a mass-based functional unit as identified in previous deliverables of the SH2E project (Ciroth et al., 2021; Bargiacchi et al., 2022; Wulf et al., 2022a; Iribarren et al., 2023). Therefore, the recommendation is to state the functional unit as a description of the **mass amount of produced hydrogen**. The functional unit must be

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accompanied in all cases with a proper definition of the reference flow. **Hydrogen purity, pressure and temperature** must be stated together with the **quantity** of produced hydrogen and the **geographical location** of the final output of the system. These characteristics are linked to important life-cycle stages such as compression and purification.

Box 11 Functional unit in systems assessing hydrogen production

1. The functional unit used in LCSAs of hydrogen production systems must represent the mass amount of produced hydrogen (e.g. kg of hydrogen).
2. Hydrogen purity, pressure and temperature, besides geographical information of the final output of the system, must be specified together with the functional unit.

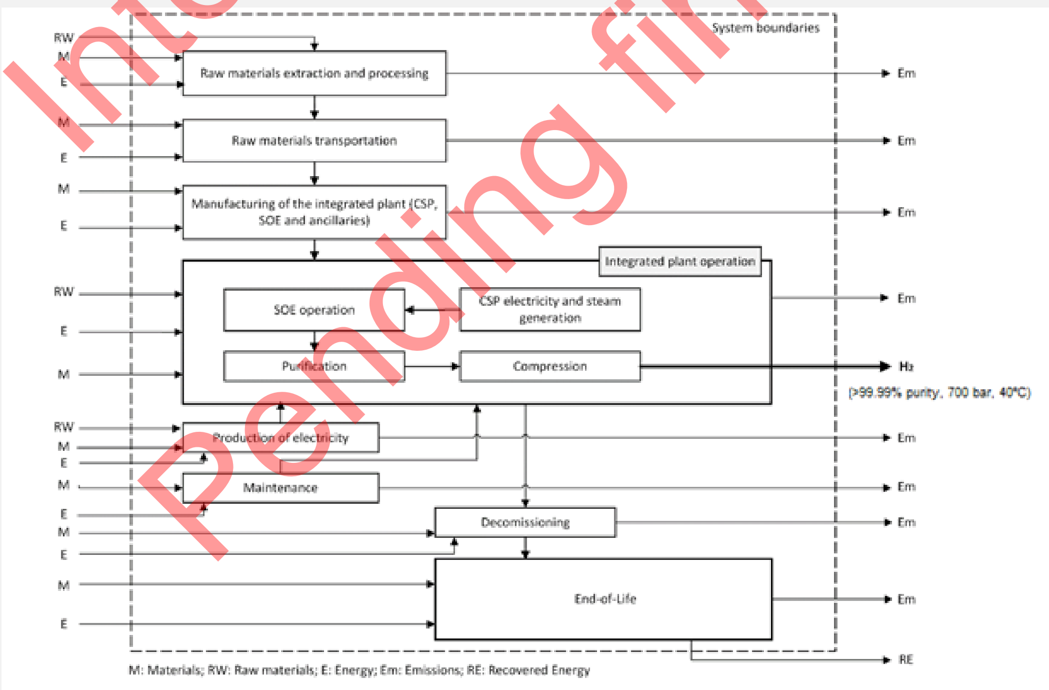
Example: (from reference [Valente et al., 2019], on LCSA and benchmarking of hydrogen production from biomass gasification)

"The two hydrogen production plants were assumed to be located in Spain […]. Both systems were assessed from feedstock production to hydrogen compression, and the functional unit (FU) was defined as 1 kg of hydrogen with 99.9 vol% purity at 200 bar and 25ºC"

Box 12 Reference flow in systems assessing hydrogen production

The reference flow, completely defined through the specification of hydrogen purity, pressure and temperature, should be indicated in the initial flow diagram of the LCSAs.

Example: (from SH2E deliverable D6.3, regarding the prospective LCSA of a high-temperature hydrogen production system)



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Requirements for Case 2: Systems including hydrogen use within the system boundaries

The heterogeneity of hydrogen applications claims for different functional units with the aim of correctly representing the function of the system. Considering that new applications for hydrogen may appear in the short and long run, this section makes general methodological recommendations. It is useful to differentiate between the system and subsystem functions. If the FCH section is a part of a larger system (e.g. **Annex 3**), a difference should be stated between the main system and subsystem functions (Bargiacchi et al., 2022; Iribarren et al., 2023).

Case 2a. Hydrogen for transportation

When hydrogen is used as a fuel for transportation, there is a general agreement on following distance-based functional units (km, p·km, t·km) depending on the specific goal of the study. The choice of a **distance-based functional unit is therefore required** since it also allows for comparison with other powertrain technologies. The specific functional unit to be selected depends on the goal of the LCSA, but a proper definition of the reference flow must be included, reporting capacity utilisation (passengers/transported freight) and the lifetime considered for the vehicle in terms of mileage. For example, the reference flow could be stated as “to travel *X* km with a fuel cell electric vehicle (FCEV) of medium size (*Y* kg) occupied by *Z* passengers with an expected lifetime range of *W* km”. The specific reference flow may include other characteristics according to the goal of the LCSA (e.g. the purity of the hydrogen required as propulsion agent), but the relationship between distance and demand (in the form of load) must always be clear. This statement is not limited to road transport, but it also includes other modalities such as air and maritime transportation.

Box 13 Functional unit in systems assessing hydrogen use for transportation

1. The functional unit employed in LCSAs of hydrogen use for transportation must represent the distance travelled for a given demand, expressed as the passenger or freight load.
2. The considered demand must be specified in the reference flow, together with the lifetime measured in terms of mileage.
3. The transportation type should be reported.

Example: (from SH2E deliverable D6.3, regarding the LCSA and benchmarking of a PEMFC passenger car)

“[…] and its use in a PEMFC passenger car. Accordingly, the functional unit is 15,000 km per year of driven distance by a single passenger FCEV for 15 years (i.e. 225,000 km of driven distance).”

Case 2b. Hydrogen for fuels and chemicals production

Hydrogen is used in multiple processes for the synthesis of chemicals and fuels. The main applications foreseen are methane, methanol and ammonia production. A functional unit that describes the produced amount must be used. The reference flow is to be specified stating the **purity, pressure and temperature of the produced chemical/fuel,** besides **geographical and temporal information** of the final output of the system.

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Box 14 Functional unit in systems assessing hydrogen use for fuels and chemicals production

1. The functional unit used in LCSAs of hydrogen use for fuels and chemicals production must represent the quantity of the produced chemical/fuel by means of a mass-based functional unit in the case of chemicals, and by either a mass- or energy-based functional unit in the case of fuels.
2. Purity, pressure and temperature of the produced chemical/fuel, besides geographical and temporal information of the final output of the system, must also be specified to guarantee a precise functional unit and fair comparisons.
3. In the case of fuels, the energy content must be clearly stated through the use of the net calorific value.

Example: (from reference [Iribarren et al., 2022], on SLCA and benchmarking of green methanol)

"The functional unit of the study was defined as 1 kg of (green or conventional) methanol produced at plant […] The green methanol system under study involves methanol production from CO_2 (directly captured from the air) and hydrogen (from wind power electrolysis) at a hypothetical plant in the USA."

Case 2c. Hydrogen for electricity and/or heat generation

Systems using hydrogen as a fuel for energy generation could be classified into electricity generation or cogeneration. The former is conceived for the production of a single product (electricity), which is the only functional flow of the system. The function of these systems is clear and an **energy-based functional unit** is required, in accordance with common practice as identified in previous SH2E deliverables (Bargiacchi et al., 2022; Wulf et al., 2022a; Iribarren et al., 2023). This energy-based functional unit must refer to the **output electricity**; thus, it **considers upstream efficiencies** (engine or fuel cell, rectifier for fuel cells, and generator). It is recommended to include and clearly state the upstream efficiencies to be able to retrieve the reference flow of the system.

Box 15 Functional unit in systems assessing hydrogen for electricity generation

The functional unit used in LCSAs of hydrogen use for electricity generation must represent the quantity of produced electricity (MJ or equivalent). Geographical and temporal information of the final output of the system must also be specified to guarantee a precise functional unit and fair comparisons. The functional unit must consider the upstream efficiencies to convert hydrogen into electricity.

For **cogeneration** systems, two functional flows appear: electricity and heat. The LCSA practitioner has to determine if heat is considered as a valuable product (functional flow) or, when not used, an emission to the environment. For the latter, the system would only be producing electricity and should follow the recommendations given in Box 15. On the contrary, when heat is a valuable product, the function of the system changes because it becomes "the production of electricity and heat". This combined function should be represented by an **exergy-based functional unit**, which represents the maximum energy potential that the system could transform into useful work (Box 16).

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Box 16 Functional unit in systems assessing hydrogen for electricity and heat generation

The functional unit employed in LCSAs of hydrogen use for electricity and heat generation must represent the maximum energy potential that the system could transform into work (i.e. exergy-based functional unit).

If heat is considered as a valuable product of the system, it is not recommended to apply allocation for comparative purposes since cogeneration would be the actual function of the system. Hence, the system should be benchmarked with functionally-equivalent systems such as combined heat and power (CHP) engines rather than addressing a separate benchmarking of each product.

This section is linked to the following sections of the present guidelines:

- 2: Goal of the Life Cycle Sustainability Assessment
- 3.4: Multi-functionality

3.3 System boundaries

Motivation

The system boundaries of an LCSA involve a set of criteria that specify which processes are included in the product system and therefore determine which unit processes shall be included in the LCSA (UNEP, 2017; Valdivia et al., 2021). They must be meticulously defined to align with the chosen goal of the LCSA. The correct identification and reporting of the chosen system boundaries are crucial, especially in the case of comparative studies.

Concerning FCH systems, a **lack of transparency regarding the flows included in the system boundaries** still persists, which often causes problems during comparison and benchmarking (Ciroth et al., 2021; Bargiacchi et al., 2022; Wulf et al., 2022a; Iribarren et al., 2023). Most of the studies include capital goods, while very few include the end-of-life (EoL) and, if so, few details are reported and a clear identification of the EoL scenarios is missing. Another specificity of FCH systems is the large variety of life-cycle phases where the study boundary might be placed, especially in studies assessing hydrogen production. In fact, after being produced, hydrogen undergoes conditioning (purification and compression), storage, transportation, and distribution before reaching the use phase. The choice of the gate largely varies depending on the specific study (Figure 1). The setting of the system boundaries in LCSA of hydrogen systems is key to ensure that the desired reference flow is achieved and, therefore, the function of the system performed.

In the context of LCSA, it is imperative that the definition of system boundaries aligns with the overarching goal. Nevertheless, it is important to acknowledge that **differences may arise in defining system boundaries across the sustainability dimensions** (LCA, LCC and SLCA) due to variations in data availability and the tools that support the development of value chains. When such differences exist, practitioners must transparently report the variations in the stages included per dimension, as well as the underlying reasons for these differences (Pihkola et al., 2022; Valdivia et al., 2021). In this way, stakeholders could clearly comprehend the differences and make informed interpretations of the results.

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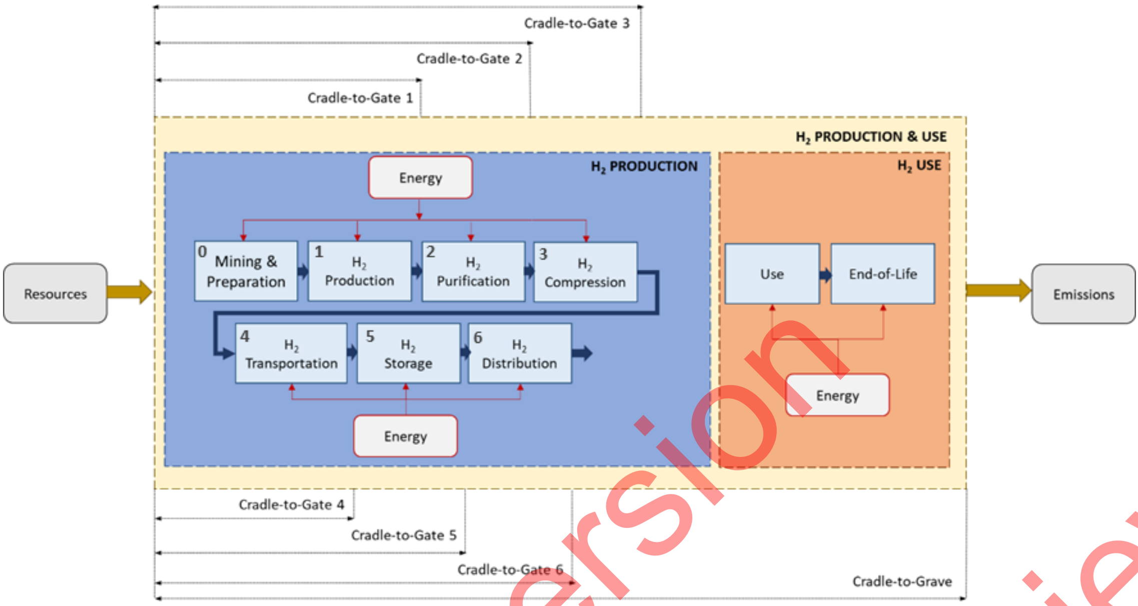

Figure 1. System boundaries for studies assessing FCH systems.

Options

Different cases are herein distinguished for the definition of FCH-specific foreground stages:

- **Case 1**: hydrogen production.
- **Case 2**: hydrogen use.
- **Case 3**: hydrogen production and use.

For case studies focusing on FCH technology manufacturing, the operational phase of the technology should be included. By doing so, this case study should match one of the three above-mentioned cases.

Requirements and recommendations

General requirements and recommendations

Box 17 System boundaries I

1. The system boundaries definition must be coherent with the goal of the study.
2. The system boundaries of the analysed system must be defined and reported.
3. The system boundaries must encompass capital goods, including their EoL phases, provide that it is feasible within the context of each sustainability dimension.

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Box 18 System boundaries II

1. Any differences in the definition of system boundaries in the embedded LCA, LCC and SLCA studies (e.g. application of different cut-off criteria) should be explicitly stated and reported to ensure transparency.
2. It is highly recommended to show the system boundaries in a flow chart.

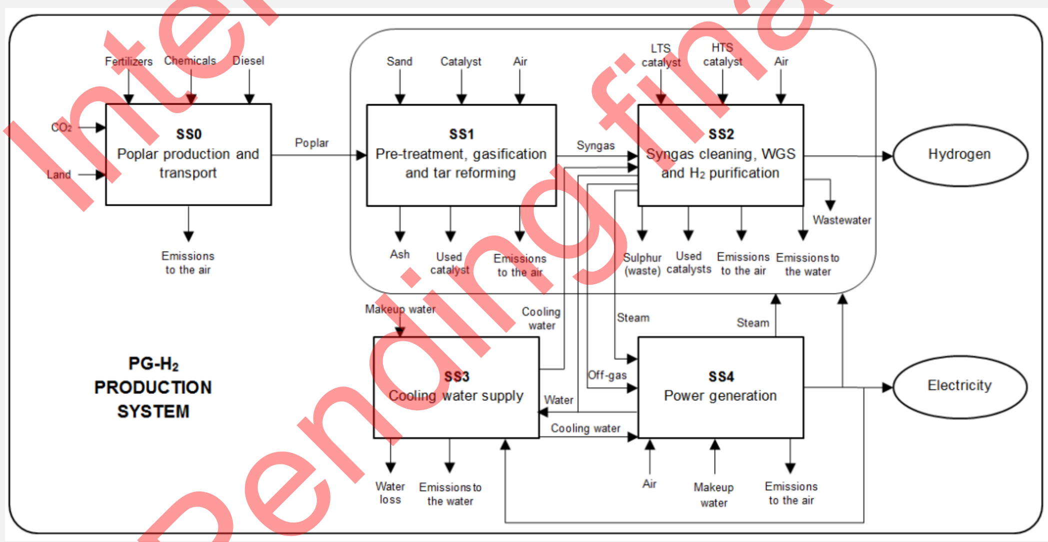
Requirements and recommendations for Case 1: hydrogen production

When conducting LCSA studies assessing only hydrogen production, the recommended system boundaries are cradle-to-gate, including hydrogen conditioning (**Cradle-to-Gate 3** in Figure 1). This recommendation assures that the produced hydrogen could fulfil the function of the system (e.g. provide high-purity hydrogen for FCEVs).

Box 19 System boundaries for systems assessing hydrogen production I

1. The system boundaries of studies on hydrogen production must be, at least, Cradle-to-Gate 1.
2. All sustainability-relevant flows must be included in the assessment. If the inclusion of flows is not homogeneous across dimensions, the reasons for variations should be reported and justified.

Example: (from reference [Susmozas et al., 2013], on the LCA of indirect biomass gasification for hydrogen production)



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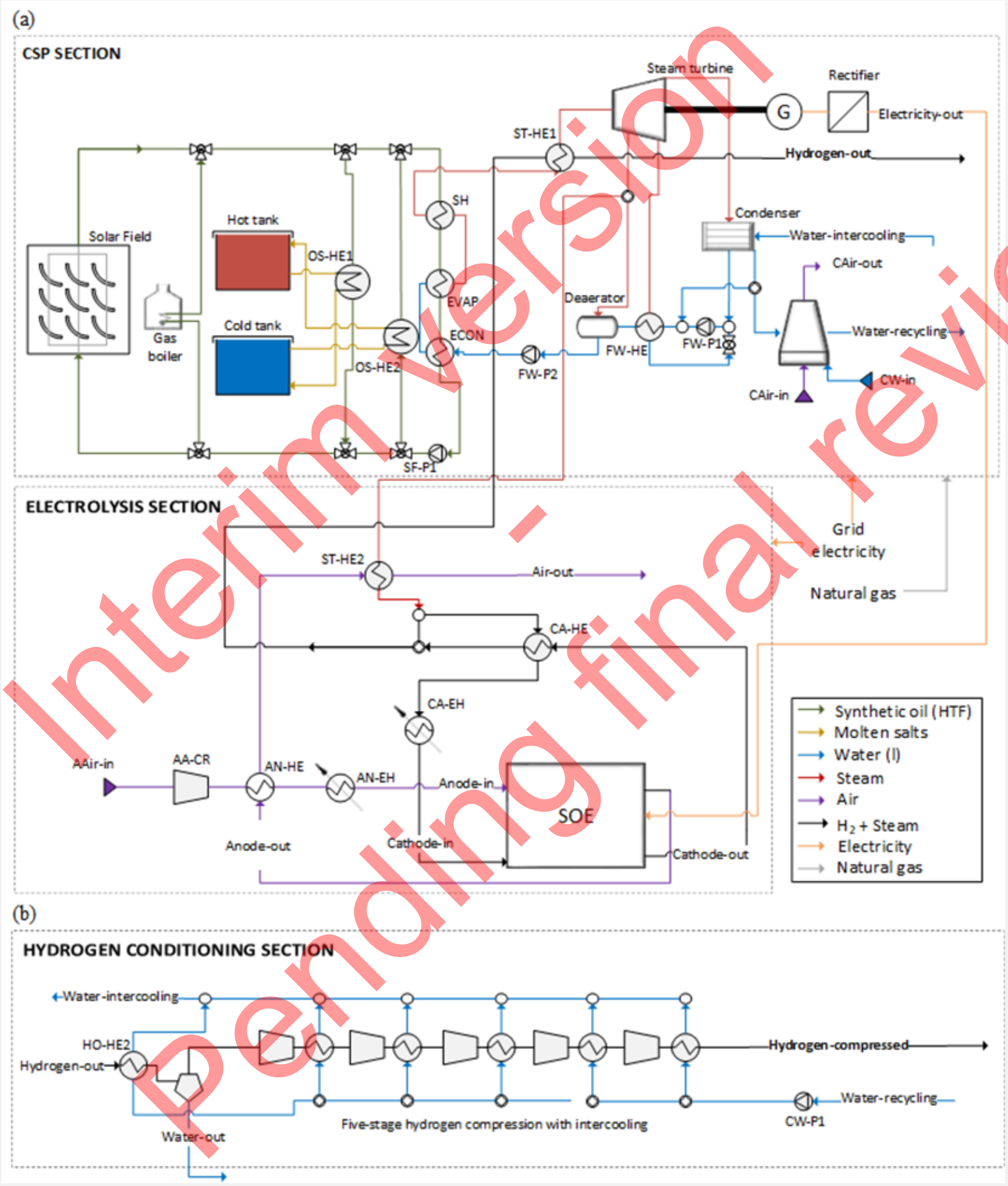
Box 20 System boundaries for systems assessing hydrogen production II

1. It is recommended to place the gate after the hydrogen conditioning section, in particular after the compression stage (Cradle-to-Gate 3).

Example: (from reference [Puig-Samper et al., 2022], on the prospective LCA of a high-temperature hydrogen production system)



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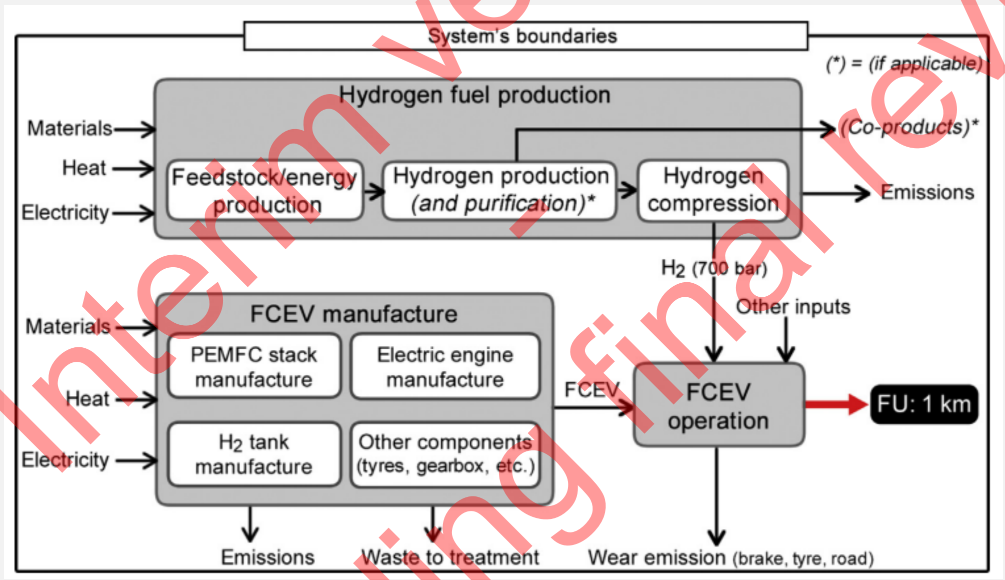
Requirements for Case 2: hydrogen use

For studies focusing on hydrogen use, it is required to carry out the LCSA study from resource extraction to the use and disposal phase (i.e. **Cradle-to-Grave**), provided that it is feasible within each sustainability dimension under study. This means that hydrogen production has to be included in the analysis, checking that the considered hydrogen is suitable (purity and pressure) for the assessed application and methodologically consistent.

Box 21 System boundaries for systems assessing hydrogen use

1. The system boundaries of studies focusing on hydrogen production must be Cradle-to-Grave.
2. All the sustainability-relevant flows must be included in the assessment. If the inclusion of flows is not homogeneous across dimensions, the reasons for variations should be reported and justified.

Example: (from reference [Valente et al., 2020], on the LCA of a PEMFC passenger car running on different hydrogen fuel options)



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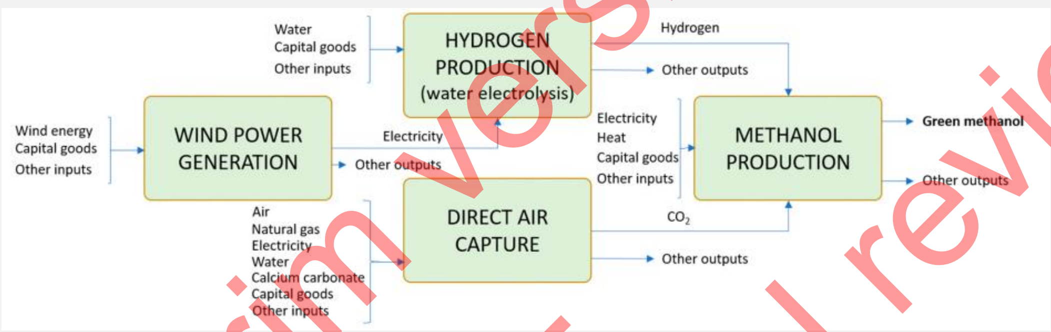
Requirements for Case 3: hydrogen production and use

When conducting an LCSA of systems for hydrogen production and use, a **Cradle-to-Grave** scope is required provided that it is feasible within each sustainability dimension under study.

Box 22 System boundaries for systems assessing hydrogen production and use

1. The system boundaries of studies focusing on hydrogen production must be Cradle-to-Grave.
2. All the sustainability-relevant flows must be included in the assessment. If the inclusion of flows is not homogeneous across dimensions, the reasons for variations should be reported and justified.

Example: (from reference [Iribarren et al., 2022], on SLCA and benchmarking of green methanol)



Requirements and recommendations to complete the FCH system: model asymmetry

The above-mentioned recommendations indicate that all relevant unit processes and flows linked to the system boundaries should be included in the assessment; if any is to be left out, a clear justification needs to be provided. For illustrative purposes, system boundaries can be understood as a set of individual background supply chains that converge vertically into its corresponding foreground phase and organised in a tier structure (Figure 2). This type of recommendation is made considering that, once the foreground system has been modelled by the practitioner, life-cycle databases on which the inventories of the corresponding background processes rely usually provide information (i.e. technosphere and elementary flows entering and leaving each block) specific to those processes. However, a significant difference exists across sustainability dimensions in the case of SLCA (Iribarren et al., 2023). Common SLCA databases typically provide information for sectors as a whole. This means the granularity and, consequently, the results are less product-specific. Nevertheless, generic data from databases could provide hints on potential social impacts. This distinction is noteworthy, as it impacts the precision of SLCA results. While generic data from these databases may not offer product-specific insights, they can still provide valuable indications regarding potential social impacts. Therefore, practitioners should be cognizant of this variation in data availability and granularity when conducting assessments across different sustainability dimensions.

Specific requirements and recommendations to complete FCH systems in SLCA studies can be found in Section 1.4 of the SH2E deliverable D4.2 on FCH-SLCA guidelines (Iribarren et al., 2023). Furthermore, the present guidelines include an example of supply-chain modelling with different scopes in SLCA (cf. **Annex 4**). This example illustrates the differences in life-

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cycle results when addressing the system boundaries with a product-specific supply chain or a sector-extended one.

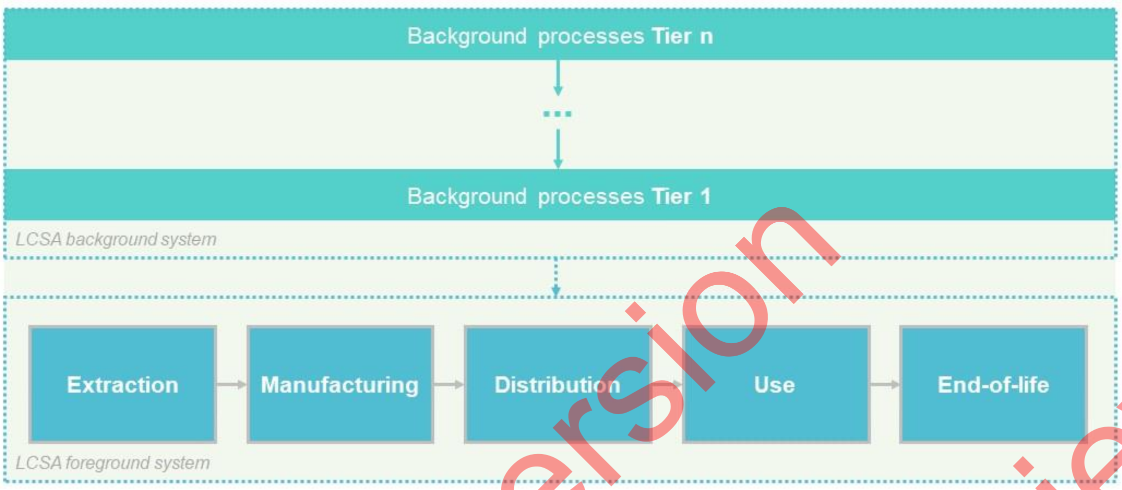

Figure 2. FCH system boundaries for LCSA.

Model asymmetry across sustainability dimensions

> *Example:*
>
> Consult **Annex 4** of this deliverable.

This section is linked to the following sections of the present guidelines:

- 3.2: Functional unit
- 3.3.1: Capital goods
- 3.3.2: Equipment end-of-life

3.3.1 Capital goods

In the context of LCSA, the role of capital goods is crucial in enabling the production of goods or the provision of services. Capital goods encompass different **physical items** necessary **for producers to manufacture the product**. At this point of production systems, the so-called **capital goods** come into effect. Even though the classification of system components as capital goods depends on the perspective of the particular study, they can be described with components such as machinery used in production processes, buildings, office equipment, transport vehicles, and transportation infrastructure (Guinee and Lindeijer, 2002; European Commission, 2013). In fact, physical items that are usually labelled as "capital goods" may become the focus of LCSA studies and thus lose their "capital goods" classification in the sense of this guidelines section. The described requirements and recommendations are still valid in such cases for capital goods needed to provide these focused products.

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Capital goods (e.g. electrolysers, compressors, etc.) **must be included** within the system boundaries, as an exclusion could lead to misleading results. Capital goods cannot be excluded per se and should be treated as any other input or output flow.

Since the usage duration often exceeds the relevant considered period of the studied goods or services, **capital goods' lifetime** (effective service life) must be taken into account. Besides the production and use of capital goods, the related **EoL activities** (cf. Section 3.3.2) shall be considered, when feasible, across the sustainability dimensions.

For reasons of transparency and completeness, comprehensive documentation regarding the consideration of capital goods must be included in the reporting of LCSA studies. Essential information includes data sources and assumptions.

Box 23 Capital goods I

To conduct LCSA studies in line with these guidelines for FCH systems, the following requirements shall be fulfilled:

1. Capital goods must be included by their phases of production, use and EoL (provided that it is feasible under the specific sustainability domain under evaluation). ●●○○○
2. The non-consideration of capital goods shall be justified by cut-off rules. ●●●●○
3. The effective lifetime of capital goods must be included. ●●●●○
4. Data sources and assumptions related to capital goods must be documented. ●●●●●

Example: (from SH2E deliverable D6.3, regarding the prospective LCSA of a high-temperature hydrogen production system)

"Capital goods involved in the foreground system under evaluation (i.e. integrated CSP and hydrogen generation plant) were included in this analysis. A detailed list of them is presented in Table 1, also documenting their lifetime and the sources from where data was collected."

For the sake of rigour and considering data availability, it is recommended to use **data with the same geographical and temporal reference for capital goods as for the other parts of the system**. For instance, this can prevent potential result-distorting influences of technology development.

Box 24 Capital goods II

When considering capital goods in LCSA studies in line with these guidelines for FCH systems, the following points are recommended:

1. Depending on data availability, it is recommended to use qualitatively appropriate data. ●●○○○
2. The geographical and time horizons considered for the capital goods should be consistent with the data used for the rest of the life-cycle phases. ●●●○○
3. The influence of capital goods on certain impact categories should preferably be highlighted in the reporting. ●●●○○

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3.3.2 Equipment end-of-life

An important topic with regard to the system boundaries is the consideration and handling of products at the end of their life. Thus, **EoL is an integral component of the product life cycle** and shall be included in LCSA modelling (Bargiacchi et al., 2022; Wulf et al., 2022a; Iribarren et al., 2023).

The end of the EoL is given when a specific flow crosses the system boundary to leave the product system (waste) or enter a new/another life cycle (Klöpffer and Grahl, 2014). Depending on the flow and EoL modelling, this endpoint can differ. In the case of including recycling or recovery processes, this point, which is usually known as point of substitution, is reached with the "outflow of recovered/recycled material". Figure 3 illustrates the general product life-cycle stages and contained activities.

EoL can lead to multi-functionality in the system, which should be addressed in accordance with Section 3.4. Thus, allocation should be avoided by system subdivision or expansion also in the EoL modelling. The modelling of EoL varies depending on the applied approach. The choice of the method has to be documented by the LCSA practitioner and requires justification. Further information about EoL modelling approaches can be found in Section 3.3.2 of the SH2E deliverable on FCH-LCA (Bargiacchi et al., 2022).

Regardless of the EoL flows fate (disposal, recycling, recovery or reuse), preparatory steps before the core EoL treatment shall be included in the modelled process chains. These activities include the collection, transport and pre-treatment (sorting, separation) of waste and reusable or recyclable material. Depending on the EoL modelling approach, these activities could be included separately from and unpaired to the core recycling and upgrading treatment (e.g. recycled content approach).

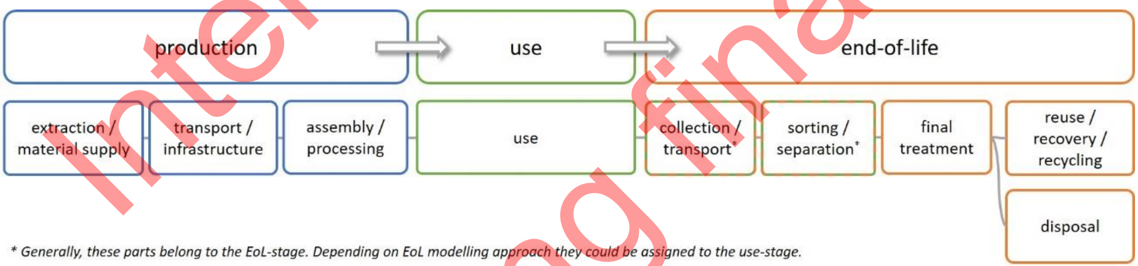

Figure 3. Simplified structure of a product life cycle with the stages production, use and end-of-life, as well as their sub-stages.

A recurring problem in cases of novel or emerging technologies EoL is the **lack of data on utilisation and disposal options**. This fact also applies to FCH-related EoL technologies and strategies. This data scarcity extends across economic and social aspects of EoL modelling, making it particularly challenging, especially when relying on life-cycle databases (Wulf et al., 2022a; Iribarren et al., 2023). In such cases, practitioners may encounter difficulties in obtaining comprehensive economic or social information for EoL modelling, creating data asymmetry across sustainability dimensions. To address data limitations, practitioners should consider various strategies. Exemplary ways of dealing with these circumstances vary from omitting the EoL phase to the **consideration of the worst-case scenario** by assuming landfilling. The latter approach was previously recommended by previous FCH-specific LCA guidelines (Bargiacchi et al., 2022). It is recommended to apply a **sensitivity analysis for at least one applicable recycling solution** to provide an estimation in the overall context. Generally, the procedure depends on the applied modelling approach. Importantly, when facing data asymmetry across sustainability dimensions, it is crucial to adopt a transparent and reasoned approach. Practitioners must recognise and

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explicitly report any differences in data availability and quality between the environmental, economic and social dimensions.

Box 25 Equipment end-of-life I

To conduct LCSA studies regarding "end-of-life" in line with these guidelines for FCH systems, the following requirements must be fulfilled:

1. The EoL of FCH technologies shall be considered, provided that it is feasible under the specific sustainability domain under evaluation. ●●○○○
2. Preparatory steps (collection, transport, pre-treatment [sorting, separation]) of EoL flows shall be considered, if not excluded by method. ●●○○○
3. Downstream activities of waste treatment, such as landfill operation and maintenance as well as ash disposal, shall be included. ●●○○○
4. The choice of the modelling approach to EoL shall be documented and justified. ●●●●○
5. System boundaries shall be drawn in line with the underlying EoL modelling approach. ●●●●●

Example: (from reference [Lotrič et al., 2021], on LCA of the manufacturing and end-of-life phases of FCH technologies)

"The LCA models for all four FCH technologies are created by modelling the manufacturing phase, followed by defining the EoL strategies and processes used and finally by assessing the effects of the EoL approach using environmental indicators […] The strategy for defining the EoL phase was divided into several steps: Manual dismantling was applied for all subsystems and components that cannot be reused. Recycling rates for different materials were defined based on data from the recycling-industry sector. Energy extraction and landfill were only used in cases where reuse or recycling was not possible, or no other data were available for the EoL."

Box 26 Equipment end-of-life II

When considering "end-of-life" in LCSA studies in line with these guidelines for FCH systems, the **following points are recommended**:

1. Depending on the modelling method, credits may be given for energy and materials recovery. ●●●○○
2. If no data are available for the waste-treatment activities, a sensitivity analysis for at least one applicable recycling solution and/or a worst case of disposal (landfilling or incineration) should be considered. ●●●○○

3.4 Multi-functionality

Motivation

Multi-functionality in LCSA is observed when a system delivers more than one functional flow. For many cases, approaches to deal with multi-functionality have been researched over the past years, and reaching a consensus in dealing with multi-functional systems is still a challenge. The hierarchy defined by ISO standards and ILCD prioritises subdivision, system

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expansion, and, in the last case, the application of allocation (International Organization for Standardization, 2006a; European Commission, 2010).

Systems producing and/or using hydrogen often lead to different outputs, and, in many cases, these outputs are considered valuable products, resulting in multi-functional processes. These guidelines propose a comprehensive approach to deal with multi-functionality for systems producing and/or using hydrogen for energy-related applications. This builds upon the individual SH2E guidelines (Bargiacchi et al., 2022; Wulf et al., 2022a; Iribarren et al., 2023).

Description of the topic

Hydrogen can be produced through different pathways, and different additional products can be obtained during its production. These products have several properties and applications, indicating the need for distinct approaches to solve the multi-functionality of the processes. Therefore, for systems producing hydrogen and other products, in which hydrogen is the quantitative reference of the modelled process in the LCSA, it is to be defined whether hydrogen is the main product or a secondary product (co- or by-product) of the studied process. For systems using hydrogen, the guidelines consider if the studied system is a fuel cell or another system using hydrogen for different applications.

Options

Different cases can be distinguished for multi-functionality:

• **Case 1**: Systems producing hydrogen.

• **Case 2**: Systems using hydrogen.

Requirements and recommendations

General requirements and recommendations

For processes delivering more than one function, it is necessary to identify the most suitable approach to solve the multi-functionality issue. For that reason, the first step is the identification/confirmation if the process can be really considered as a multi-functional process, through the **identification of the functional** and non-functional **flows** (Box 27). For instance, if, besides the product flow, all the output flows are elementary flows, then it is not a case of multi-functionality, as elementary flows (resources/emissions from/to nature) are not considered functional flows.

> **Box 27 Multi-functionality I**
>
> It must be identified if the investigated process is a case of multi-functionality or not through the identification of the functional flow(s).

In the event that the studied process is identified as a multi-functional one, then the **ISO 14040/14044 recommendation** shall be applied, according to Box 28 (International Organization for Standardization, 2006a, 2006b). Therefore, allocation should be avoided by applying subdivision or system expansion, if possible. In case allocation cannot be avoided, then the relationship between functional flows should be studied for the definition of the allocation factors. However, it is essential to recognise that certain limitations may arise in the harmonisation of multi-functionality across sustainability dimensions.

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In instances where allocation cannot be entirely avoided, practitioners should exercise caution, particularly in the context of LCC where multi-functionality shall be solved by applying subdivision or system expansion (Wulf et al., 2022a). When facing such situations, it becomes crucial to transparently **acknowledge and explicitly state any differences in the application of multi-functionality across sustainability dimensions**. This serves to prevent misunderstandings and enhances the overall transparency of the LCSA study.

Box 28 Multi-functionality II

1. In case of multi-functionality, allocation needs to be avoided by the application of division of unit processes into different sub-processes, according to the outputs produced.
2. Another alternative to avoid allocation is, when appropriate, the application of system expansion.
3. If allocation cannot be avoided, allocation must be applied partitioning inputs/outputs according to the physical relationships between them or other possible relationship (e.g. economic).
4. The multi-functionality approach selected by the LCSA practitioner must be consistent across sustainability dimensions. Any differences must be transparently acknowledged, explicitly stated and justified.

Example: (from reference [Valente et al., 2021], on comparative LCSA of renewable and conventional hydrogen)

"On the other hand, in hydrogen production from biomass gasification (BMG_H), the PSA off-gas is employed to produce electricity, which is partly used to satisfy the internal electricity demand while the surplus was assumed to be sold to the Spanish electricity grid. Hence, besides hydrogen production, the BMG_H system presents the additional function of electricity coproduction, which was addressed through systems expansion by displacing the production of the Spanish grid electricity mix and the corresponding burdens. In contrast, no additional functions are associated with the other systems for hydrogen production."

Requirements and recommendations for systems producing and/or using hydrogen

Following the general recommendations, first, it must be identified if the other outputs of the process are, in fact, functional flows (Box 27). In case they can be considered emissions to nature (e.g. in many processes oxygen as an output can be regarded in this way), then elementary flows should be selected, indicating that it is not an actual case of multi-functionality. If the output can be considered a waste of the process, then a waste flow should be applied, and the waste treatment process should be selected. However, if the outputs are indeed considered product flows, this indicates that one of the approaches defined by the ISO 14040/14044 hierarchy should be applied (Box 28). The particularities arising from each case (systems producing and using hydrogen) are detailed in the next paragraphs.

As outlined in the individual SH2E life-cycle guidelines (Bargiacchi et al., 2022; Wulf et al., 2022a; Iribarren et al., 2023), it is recommended to explore the effect of the approaches to deal with multi-functionality through **sensitivity analysis** (Box 29).

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Box 29 Sensitivity analysis and multi-functionality

Additionally, it should be considered that:

1. Sensitivity analysis is recommended in order to compare the different approaches to deal with multi-functionality and explore the influence of subdivision (if possible), system expansion, and allocation on the results.
2. Sensitivity analysis to investigate the effects of economic values oscillation is also recommended for economic allocation.

Case 1. Systems producing hydrogen

Following the general recommendation, the first possibility to solve multi-functionality for systems producing hydrogen is the application of **subdivision** (Box 30), which is in many cases not possible, as usually the same processes deliver different products. The second step in the hierarchy is the application of **system expansion** for the other products (Box 30). To select the alternative system, allowing to account for the credits of system expansion, it must be identified if hydrogen is the main product from an industrial perspective, and if there are other possible processes producing the other outputs. System expansion is not always possible, as sometimes it is challenging to define an alternative process. For instance, system expansion may not be possible for systems producing hydrogen in which hydrogen is considered the by-product of the process from an industrial perspective (e.g. steam cracking or chlor-alkali electrolysis).

Following the ISO standard hierarchy, the next possibility would be the application of **allocation** (Box 30). When dealing with hydrogen, it must be considered that mass allocation is not recommended as this would associate a low ratio of the impacts to the hydrogen production. Hence, the first recommendation when applying allocation is the use of physical allocation using the energy content (clearly stating the energy basis; e.g., lower heating value). However, this is not possible for many secondary products. If considering the energy content is not feasible, due to the characteristics of the obtained products, then physical allocation based on number of moles is suggested. Otherwise, prioritising non-physical allocation (e.g. economic allocation) is recommended (Box 31).

Economic allocation is suggested for the cases in which the previous alternatives are not representative of the system and/or where the economic aspects of the products are particularly relevant. The economic values selected should be from the same studied region. In addition, the investigation of price oscillations over the past two years should be considered through a sensitivity analysis if relevant. Finally, if economic aspects are not relevant to distinguish the different outputs of the process, then the recommendation is the application of physical allocation based on the mass (Box 31). Further information about the choice of allocation factors for hydrogen systems are provided in the individual SH2E life-cycle guidelines: Section 3.4 and Section 1.7 of the SH2E deliverables D2.2 (Bargiacchi et al., 2022) and D4.2 (Iribarren et al., 2023), respectively.

To ensure that **multifunctionality is addressed consistently across sustainability dimensions**, a hierarchy for handling multi-functionality is applied. However, the hierarchy may vary depending on the dimension:

1. For environmental LCA and SLCA, the hierarchy includes:
   - Subdivision
   - System expansion
   - Allocation

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2. For LCC, the hierarchy simplifies to:
   - Subdivision
   - System expansion

In all cases, sensitivity analyses are recommended to investigate and compare the different approaches to deal with multi-functionality.

Box 30 General decision flow for multi-functionality in LCSA of hydrogen production systems

1. The multi-functionality approach selected by the LCSA practitioner must be consistent across sustainability dimensions. Any differences must be transparently acknowledged, explicitly stated and justified.
2. Subdivision must be preferred.
3. If subdivision cannot be applied, system expansion is the second preferable option.
4. If it is not possible to apply system expansion in environmental LCA and SLCA, physical allocation based on energy content needs to be applied when only energy (-carrier) products are involved. If not possible, physical allocation based on number of moles must be selected. Otherwise, economic allocation is suggested. If there is no economic relevance or the previous alternatives are not possible, mass allocation should be applied, and the limitations of this application should be stated. If the recommended allocation methods are not suitable for the investigated system, allocation factors should be defined based on causal relationships or activity variables, such as worker hours or added value.

Case 2. Systems using hydrogen

One of the most common hydrogen applications is in fuel cells. Fuel cells generate electricity and heat, which can be considered both valuable products in many cases. Therefore, this would represent a case of multi-functionality. The produced water is usually not a functional flow, since it can be modelled as a waste. For fuel cells, it might be not possible to apply **subdivision**, as the same system is generating both electricity and heat. On the other hand, sometimes **system expansion** can also involve concerns on the identification of a representative alternative for heat production. Regarding the application of **allocation**, exergy should be defined as the functional unit and the reference for allocation (Box 31). If it is not possible to apply physical allocation based on exergy, then economic allocation should be applied (Box 31).

The approach to manage multi-functionality should consider the **sustainability dimension being evaluated**:

1. For environmental LCA and SLCA, the hierarchy to address multi-functionality consists of:
   - Subdivision
   - System expansion
   - Allocation (exergy-based allocation and, if not feasible, economic allocation)
2. For LCC, the hierarchy simplifies to:
   - Subdivision
   - System expansion

The different approaches to deal with multi-functionality should be investigated through **sensitivity analysis**. Sensitivity analysis to investigate the effects of economic values oscillation is also recommended for economic allocation.

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It is important to emphasise transparency and clarity when addressing potential differences across sustainability domains. These differences should be clearly acknowledged, justified and reported. If heat is not a valuable product, it should be modelled as an emission to the environment (therefore an elementary flow, and not a case of multi-functionality); the water produced in fuel cells can also be modelled as an elementary flow.

Box 31 Fuel cells and multi-functionality

For fuel cells constituting a case of multi-functionality, in case physical allocation is applied, exergy must be applied for the calculation of the partitioning factors between electricity and heat. If it is not possible to apply physical allocation, economic allocation is the second alternative for the definition of the allocation factors.

For all the other cases with systems that apply hydrogen for the most distinct functions, the general recommendations for multi-functionality should be respected, and sensitivity analysis to investigate the different approaches and compare their effect on the results is recommended.

Evaluation: "method readiness level"

The approach on how to handle multi-functionality in LCSA is the following:

- Identification of multi-functionality ●●●●●
- Dealing with multi-functionality in systems producing hydrogen ●●●●○
- Dealing with multi-functionality in systems using hydrogen ●●●○○

This section is linked to the following sections of the present guidelines:

- 3.2: Functional unit
- 3.3: System boundaries

3.5 Materiality assessment and stakeholder engagement

The range of topics to address within an LCSA is wide. Many important aspects in all three dimensions including environment, economy, and social aspects, exist, but sometimes not all of them can be addressed at the same time. Key topics for the goal of the study have to be identified and prioritised in order to generate a set of indicators that suitably reflects the goal of the LCSA study. In addition, also the system boundaries have to be drawn in a way that all relevant unit processes are included, i.e., the processes that affect one of the three LCSA dimensions minimum (Valdivia et al., 2021).

A concept addressing these issues is **materiality assessment**, originally stemming from accounting and its reporting requirements (Bean and Thomas, 1990). According to the Global Reporting Initiative (GRI, 2023a), material topics "[…] are topics that represent an organization's most significant impacts on the economy, environment, and people, including impacts on their human rights." The UNEP guidelines for SLCA (UNEP, 2020) define materiality assessment as "[…] a process to select topics that are more important because of their impact on stakeholders and/or on the business."

The definitions reveal the two-sidedness of the concept, what is called double materiality. GRI (2022) and the directive for corporate sustainability reporting of the European Union (2022) distinguish between financial materiality and impact materiality. **Financial materiality** entails information relevant to investors, e.g., on value creation, development and

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performance of the organisation, also including how sustainability aspects (i.e. risk from a sustainability point of view) affect the organisation. On the other hand, **impact materiality** is about information for various stakeholders, e.g., next to investors, also customers, employees, suppliers, and local communities. The impacts incorporate the economy, environment and people including topics as human rights, anti-corruption, and bribery.

GRI (2023a) has set up a procedure to identify material topics. The first step is to get an understanding about the context of the own business, including the business activities, business relations, sustainability aspects, and stakeholders. In a second step, the actual and potential impacts, positive and negative ones, are identified. This can be conducted by information from different sources, e.g., financial audits or health and safety inspections. Also documents from the Organisation for Economic Cooperation and Development (OECD) can be conducted, e.g., the OECD due diligence guidance for responsible business conduct (OECD, 2018) or sectoral guidance (OECD, 2023). In the third and last step, the significance of the impacts is assessed, e.g., how severe they are and the probability of their incidence. The sector standards by GRI can support all of these steps. More information can be found in their universal standard (GRI, 2023a).

For LCSA, the GRI procedure as well as the GRI sector standards can help practitioners identify **material topics**. Even though GRI standards are not available for every sector, this does not contradict their procedure, which can still be followed through GRI (2023a, 2023b). While no standard exists for the hydrogen sector, the oil and gas sectors serve as an example. Within this sector standard, 22 material topics are stated, including environmental topics, e.g., air emissions, biodiversity and waste; economic topics like asset integrity or economic impacts; and social material aspects, e.g., health and safety, forced labour and modern slavery (GRI, 2023c).

The LCSA-related ORIENTING framework states that materiality assessment can be built upon literature, e.g., previous studies, sector guidelines, reports or stakeholder consultations and own estimations (Pihkola et al., 2022). They provide several guiding questions which help with the identification of material topics, including (Pihkola et al., 2022):

- “What are the raw materials included in the product’s life cycle (including packaging materials)?
- What is the origin of those raw materials?
- Are any of the raw materials critical according to the European Commission’s list of Critical Raw Materials (CRMs)? […]
- Do you have any data, measurement or quantified knowledge of circularity actions in place that retain the value of the product, its parts, or materials?
- Do you know what type of environmental, economic and social impacts are or could be related to different life cycle stages?
- Do you have any measured information, data or other evidence or knowledge about the impacts that might take place in other stages of the life cycle? Is it possible to collect such data from suppliers, other actors or from statistics?
- What type of environmental, social or economic risks could be related to the different life cycle stages? Are there any processes or measures in place for mitigating such risks?”

The relation of materiality assessment and stakeholders is twofold. With the help of a materiality assessment, relevant stakeholders to address within the social dimension of an LCSA can be identified, e.g., different stakeholder groups like workers, the local community or society. However, also using stakeholder consultations as a starting point for materiality assessment, as stated above, is possible.

If relevant stakeholders are to be selected, focus groups can help (UNEP, 2020). In addition, expert judgements, literature and the availability of data are points to include in the selection

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(Tragnone et al., 2022). Also, participatory approaches are a useful tool. They divide stakeholders into two groups: directly affected and involved stakeholders, and external stakeholders. With the help of questionnaires, stakeholders have the chance to provide priorities for sustainability topics and, by doing so, add to the materiality assessment (Bouillas et al., 2021).

Several ways to identify material topics exist. Practitioners can choose the best fitting option for the entity to be assessed and its available resources, e.g., depending on whether a disclosure for financial and sustainability reporting is in place (and if it follows, e.g., the GRI guidelines), if there are established ways to communicate with different stakeholders, etc. The materiality assessment, in either case, must be conducted in a transparent manner, which makes the process comprehensible and reliable.

Evaluation: "method readiness level"

- Consideration of the application of materiality assessment in LCSA ●●●●○

This section is linked to the following sections of the present guidelines:

- 2: Goal of the Life Cycle Sustainability Assessment
- 3: Scope of the Life Cycle Sustainability Assessment

3.6 Final remark

It should be noted that certain aspects of the goal and scope included in the individual SH2E life-cycle guidelines, such as considerations related to **biogenic carbon** in environmental LCA and **discounting** in LCC, are highly specific to their respective methodologies/dimensions. Due to the specialised nature of these topics, detailed information can be found in Section 3.5 of the SH2E deliverable D2.2 on FCH-LCA (Bargiacchi et al., 2022) and in Section 3.1.3 of the SH2E deliverable D4.1 on FCH-LCC (Wulf et al., 2022a). Additionally, an illustrative example regarding modelling of a biogenic carbon balance can be consulted in **Annex 5**.

4. Life Cycle Inventory

4.1 Activity and intensity

In LCA, an **activity** refers to an individual process, operation or action that is involved in the life cycle of the product system. Activities are identified and described in the LCI phase of an LCA study, where data related to inputs and outputs for each activity are collected and quantified. In the case of **intensity**, this is a measure used to quantify the impacts associated with a specific activity (European Commission, 2010). In the context of an LCSA study, some distinctive characteristics can be found across sustainability domains.

In **environmental LCA**:

- At the LCI stage, each activity is assigned several inputs and outputs (International Organization for Standardization, 2006a, 2006b). Those from and to the biosphere, conceived as natural substances that are called elementary flows, are the native drivers of the environmental impacts corresponding to the activity. Some examples of such elementary flows are CO_2 emitted into the air or copper extracted from the ground.
- At the LCIA stage, each elementary flow, at each individual impact category, is characterised by an intensity factor (i.e. characterisation factor). An example of characterisation factor for the climate change impact category (as defined in the Environmental Footprint method) is the 1 kg of CO_2-eq assigned to the mass unit of CO_2 emitted by a process.

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In **LCC and SLCA**:

- While the concepts in LCC are analogous to environmental LCA, with the particularity of monetisation as intensity, the concept of activity becomes more intricate in SLCA. For instance, in type I SLCA, the activity variable more commonly used (i.e. worker hours) is to be assigned a qualitative risk level that determines which intensity factor applies to it afterwards (UNEP, 2020). Moreover, this risk level varies depending on the social indicator that is aimed to be assessed. In this sense, the intensity concept merges into the LCI stage, turning an a priori single activity variable type (i.e. worker hours) into a wider set defined by the qualitative attributes that emanate from the impact assessment phase (e.g. worker hours; child labour indicator; high risk). The present guidelines include an illustrative discussion of social database implementation with and without activity variable (**Annex 6**).

The distinctive feature of LCSA is the integration of the environmental, economic and social dimensions into a single assessment framework (Valdivia et al., 2011). In this context, the separation between activities and intensities can become less clear, especially in SLCA. It is essential to recognise that this integration inherently involves data asymmetry, whereby data sources and data granularity may vary significantly across sustainability dimensions. In light of this, clear and transparent reporting of data sources for both activities and intensities becomes paramount to ensure the reliability and reproducibility of LCSA results (Valdivia et al., 2021).

4.2 Data sources and availability

The essence of LCSA is rooted in acknowledging and addressing data asymmetry along the three common sustainability dimensions, and it underscores the need for open and comprehensive documentation of data sources and quality. This practice is crucial to advance the understanding of the sustainability impacts of FCH systems while fostering robust, transparent, and data-driven assessments across the environmental, economic and social facets of sustainability.

Box 32 Data sources traceability

Every data source must be clearly stated (thus ensuring data traceability), and an assessment of transparency and credibility is recommended.

For LCSA, there are no additional data sources foreseen, as LCSA is an integration of the results obtained in LCA, LCC, and SLCA. The share of foreground data can of course be addressed. For environmental LCA, an evaluation table for foreground data sources has been developed and is described in the FCH-LCA guidelines (Bargiacchi et al., 2022). This evaluation table is also applicable to data sources used in LCC and SLCA. Often, however, all three dimensions will share one inventory, and thus the processes will be shared as well, which, in turn, will make a repeated assessment of the same processes in different sustainability dimension not very meaningful. As system boundaries in the three dimensions will be equivalent but not necessarily identical, some processes may remain to be evaluated in LCC and SLCA. It is therefore recommended to apply the table provided in the environmental FCH-LCA guidelines (Bargiacchi et al., 2022) to all processes used in the LCSA inventory.

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4.3 Data quality

Motivation

Just like for each of the single life-cycle methods, it is also interesting in LCSA to understand how far the considered information fits to the decision at stake. Hence, data quality addresses how well information fits to stated requirements, and thus, for example, to a decision.

Description of the topic and key terms

For LCA, LCC and SLCA, a common approach and structure for assessing data quality was proposed in the respective guidelines, using the **pedigree matrix approach**, with slight customisations tailored to the specific sustainability dimension (Bargiacchi et al., 2022; Wulf et al., 2022a; Iribarren et al., 2023). As recommended in each set of guidelines per each aspect, the aggregation of data quality scores should be executed on a per-indicator basis throughout the product's life cycle, meaning that the result is a final, aggregated score per data quality indicator, over the life cycle, for each of the sustainability dimensions.

In LCSA, therefore, a key task is to seek for **harmonisation**, and to aggregate these data quality results, towards one sustainability data quality. Since all data quality assessments in the different dimensions follow the same principles, it can be assumed that they fit together, and are consistent and sufficiently harmonised, so that they can indeed be aggregated.

For the aggregation, different pathways can be conceived (Figure 4):

- First, per dimension. Here, data quality scores are aggregated over impact categories and over the different quality indicators, per sustainability dimension. Afterwards, results for the three sustainability dimensions are aggregated into one final data quality result. This is shown in the upper half of the figure.
- A second option is to aggregate initially overall impact assessment categories, keeping the results per data quality indicator separate. This is shown in the bottom part of the figure (1 in the figure). This result can be further aggregated, either via the data quality indicators, keeping the impact categories separate (2a in the figure), or via the impact categories, keeping the quality indicators separate (2b). These two results can be further aggregated into one final aggregated data quality result in steps 3a or 3b.

Next to decide are the “mechanics” of the **aggregation** in each case (i.e. the aggregation formula) and also the weights when aggregating across sustainability dimensions, or also across different impact categories in one sustainability dimension. This topic has already been addressed several times in literature, e.g., by Greco et al. (2019) and Wulf et al. (2023), without one clear recommendation especially for hydrogen systems. For SH2E, it is recommended to apply the same weighting as in the result calculation itself.

Rules for the aggregation across data quality indicator cannot be taken from the result calculation, as these data quality indicators are specific to data quality. There is much less literature about this topic. For now, it is recommended to let users decide about weights, address them in goal and scope, and apply these then in the aggregation.

For the aggregation of data quality scores apart from the weights, a simple arithmetical average can be applied (a). An alternative is to take the square root of the sum of squared scores (b). Scores commonly used for data quality assessment (Bargiacchi et al., 2022; Wulf et al., 2022a; Iribarren et al., 2023) range from 1 to 5, with 1 being best. The aggregation with squares puts more emphasis on extremes, as small values get very small, and values above one become large. This means that with the squared aggregation, unfavourable scores will be emphasised.

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Finally, the number format of the scores resulting from the aggregation needs to be specified. In the original pedigree approaches (Funtowicz and Ravetz, 1990; Ciroth, 2004) the scores are always full numbers. This is typically motivated by the idea of pedigree as a rough classification, which best fits to an ordinal result, which can even be re-translated into text (very good, good, etc.). In contrast to this, in the environmental footprint, scores remain as they are calculated, and thus are commonly reported with two decimal places. For the SH2E methodology, it is recommended to provide, as an option, also the fully calculated results, with two decimal places.

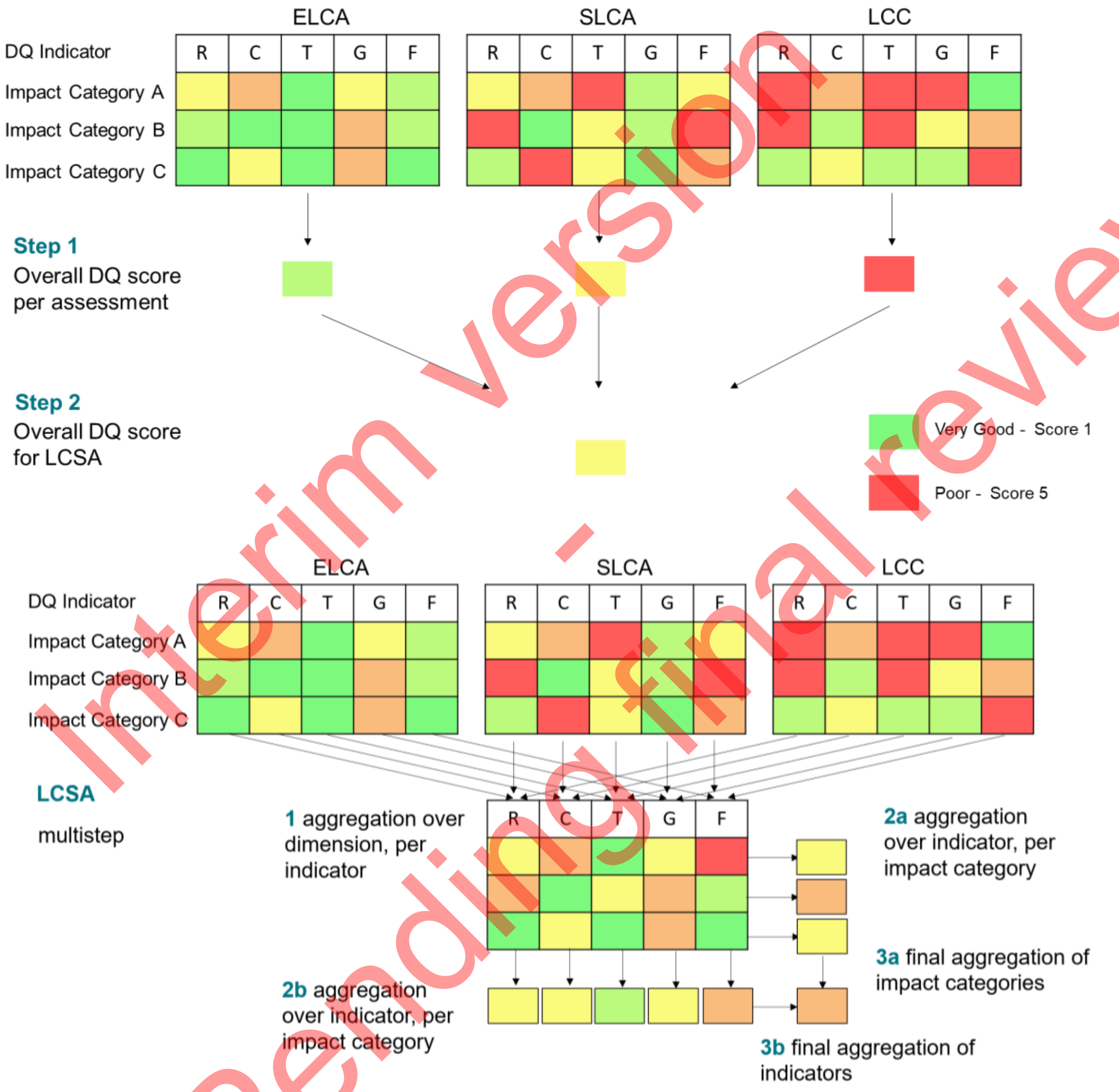

Figure 4. Data quality aggregation in LCSA.

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Box 33 Data quality I

Data quality must be documented and a data quality system with different data quality indicators must be applied for LCSA studies in general and about hydrogen systems specifically.

> *Example:* (from SH2E deliverable D6.3, regarding the LCSA and benchmarking of a PEMFC passenger car)
>
> "The quality of all flows and processes was assessed in the software openLCA, using the ecoinvent data quality system. For the background processes, the ecoinvent data quality system was also applied."

Box 34 Data quality II

Data quality must be considered for unit process datasets, for exchanges, for aggregated data sets, and for calculation results and studies.

Further information about data quality indicators for hydrogen systems are provided in the individual SH2E life-cycle guidelines: D2.2 Section 4.2 (Bargiacchi et al., 2022), D4.1 Section 4.3 (Wulf et al., 2022a), and D4.2 Section 2.2 (Iribarren et al., 2023).

Evaluation: "method readiness level"

- Data quality assessment ●●●○○

This section is linked to the following sections of the present guidelines:

- 2: Goal of the Life Cycle Sustainability Assessment
- 3: Scope of the Life Cycle Sustainability Assessment
- 4.1: Activity and intensity

4.4 Data verification and validation

It is important to try to ensure that the assessment model is good and correct, and that the model assesses what it should. **Verification** is the procedure to ensure that the assessment is correctly executed, and the assessment model correct; validation is the procedure to ensure that the model assesses what it should (Ciroth, 2006).

Verification focuses on the technical execution. As the entire LCSA involves many steps, also many steps could be executed in an incorrect way, which leads to, when executed, a failed verification. To successfully pass a verification, therefore, a combination of several points is needed or at least desirable:

- **Verification of input data** (for processes used in life-cycle models, for the life-cycle model itself, in the sense that the connections set in the models are not incorrect, for impact indicators, and for weighting factors).
- **Verification of calculation routines**; it is recommended to implement the developed approach in software, and verify the software, so that calculation routines are executed in an identical way, each time.

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- A support for users to follow the developed approach, with wizards in the software, but also with **guidelines**.
- Some aspects can also be verified in combination.

This verification needs to be performed only once for some points, but for others, each single model and assessment should undergo a verification. This deserves more exploration, but in short, generic input data and the software tool need to be verified only once. User modelling actions are case-specific and thus need to be verified per case. One can imagine a development similar to environmental product declarations, EPDs according to ISO 14025.

Validation is a "deeper" term than verification. One can assume that LCSA should model the sustainability of a system over its life cycle in a correct way. Sustainability, however, is in its common definition not easy to operationalise. It would require an assessment of the stability of the analysed system under stress. This analysis is possible with system dynamics models, which go beyond the scope of the SH2E project. Nevertheless, the deliverable D2.2 on FCH-LCA guidelines contains a reference and short explanation (Bargiacchi et al., 2022).

Within these FCH-LCSA guidelines, we can simply state that the LCSA model should model the life cycle of hydrogen systems in a correct way, for all three sustainability dimensions, and provide an aggregated result for the "total" sustainability of the investigated system. With this definition and understanding, verification and validation are congruent, and thus it suffices to verify the LCSA model.

5. Life Cycle Impact Assessment

Motivation

The LCIA phase builds on the inventory and calculates the indicators representing different sustainability impacts (International Organization for Standardization, 2006a; UNEP, 2017). It is important to align the selection of impact assessment methods with the study's goal, while ensuring that the chosen impact categories are based on a thorough **materiality assessment**. It is crucial to **avoid an imbalance** in the evaluation of the three dimensions of sustainability by carefully considering the number of indicators. The consideration of criticality as an additional sustainability aspect is recommended. Information on criticality implementation is available in Bargiacchi et al. (2022), Zapp and Schreiber (2021) and **Annex 7**.

Box 35 Life Cycle Impact Assessment

In accordance with the goal and scope of the LCSA study, the selected impact assessment methods with the corresponding impact categories must be stated and justified through a materiality assessment that incorporates the perspective of the stakeholders.

5.1 Evaluation methods

To facilitate a comprehensive understanding of LCIA methods, this section compiles the main features of the individual methods per sustainability dimension.

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Environmental life cycle impact assessment method and categories

Box 36 Environmental life cycle impact assessment method and categories

As part of the scope of the LCA, the selected impact assessment method with the impact categories must be included and justified. As for any LCA, compatibility between the inventory flows and the flows applied in the calculation method must be verified. The use of the latest version of the Environmental Footprint method (prepared by JRC) is required (currently version 3.1), and the impact categories based on a materiality assessment. In case it is decided not to include a specific impact category, this must be justified. The characterisation factors provided by the method provider should be checked.

Example: (from SH2E deliverable D6.3, regarding the prospective LCSA of a high-temperature hydrogen production system)

"The Life Cycle Impact Assessment (LCIA) method selected for the study was the Environmental Footprint version 3.1 (EF 3.1, latest available), developed by the Joint Research Centre (JRC) and recommended "as a common way of measuring environmental performance" by the European Commission."

Economic life cycle impact assessment method and indicators

Box 37 Economic life cycle impact assessment method and indicators

The calculation method used for the life cycle costing of FCH products must be clearly stated and defined.

- In case of hydrogen production, the LCoH indicator (levelised cost of hydrogen) must be used (expressed in economic units per functional unit, e.g., €/kg H_2).
- In case of hydrogen use in mobility applications, the TCO indicator (total cost of ownership) must be used, expressed in economic units per functional unit (€/p·km if the main function is the transport of passengers or €/t·km if the main function is the transport of goods).

Example: (from SH2E deliverable D6.3, regarding the prospective LCSA of a high-temperature hydrogen production system)

"The LCoH indicator was calculated, as required by the SH2E LCC guidelines for hydrogen production systems. The formula specified in the guidelines was applied, and the value of cost of capital (r) was assumed to be equal to the discount rate of 5% […] The LCoH from SOE is 7.64 €$_{2023}$/kg of hydrogen."

Clean Hydrogen Partnership

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Social life cycle impact assessment method and categories

Box 38 Social life cycle impact assessment method and categories

The calculation method used and the social indicators for the SLCA of FCH products must be clearly stated and defined. It is required to use the Reference Scale Approach (Type 1) for the assessment of FCH systems, while the impact categories to be assessed must be in line with the goal of the study and the materiality assessment. In this sense, a transparent description of the justification of impact category selection must be included.

Example: (from SH2E deliverable D6.3, regarding the prospective LCSA of a high-temperature hydrogen production system)

"The Social Life Cycle Impact Assessment (SLCIA) method selected for the study was the PSILCA method [29]. […] The impact categories specifically assessed in this study are "child labour", "contribution to economic development", "fair salary", "forced labour", "discrimination" and "health and safety."

Further information about the specific impact assessment methods are provided in the individual SH2E life-cycle guidelines: Section 5 of the deliverables D2.2 (Bargiacchi et al., 2022) and D4.1 (Wulf et al., 2022a), and Section 3 of the deliverable D4.2 (Iribarren et al., 2023). Finally, it should be noted that certain aspects of the impact assessment in the individual guidelines, such as considerations related to **non-linearity, risk assessment, and externalities**, are highly specific to their respective methodologies. Due to the specialised nature of these topics, detailed information can be found in above-mentioned sections.

Evaluation: "method readiness level"

- Selection of impact assessment method ●●●○○
- Selection of impact categories ●●●○○

This section is linked to the following sections of the present guidelines:

- 3.1: Modelling approach
- 3.2: Functional unit
- 3.3: System boundaries
- 4.1: Activity and intensity

6. Interpretation and final remarks

Motivation

All results from the study need to be discussed in depth, constituting a basis for conclusions, recommendations, and decision-making in accordance with the goal and scope definition. The analysis of results includes several steps to check aspects such as completeness, consistency and sensitivity, also entailing the conclusion, limitations and recommendations of the study (Valdivia et al., 2021).

Description

Within the **completeness check**, the requirements from the goal and scope phase are checked against their implementation in the inventory and the impact assessment. All objectives that could not be achieved, as well as the respective reasons for it, are identified

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and can be complemented through the iterative nature of the LCSA methodology. If it cannot be complemented, the goal and scope should be updated.

The **consistency check** places the focus on data from the inventory and the impact assessment and answers the question whether they are unambiguous and in line with the goal and scope.

Box 39 Interpretation

The interpretation should include completeness check, consistency check, sensitivity analysis, and conclusion with limitations and recommendations.

6.1 Sensitivity and uncertainty analysis

Sensitivity analysis is a systematic approach that is used, within the LCSA context, to assess the influence of changes in input parameters, assumptions (cf. **Annex 8**) or data on the impact results of the study (Wei et al., 2015). In this way, by conducting a sensitivity analysis, LCSA practitioners are in position of identifying which are the most relevant factors of an LCSA study and focus resources on enhancing their accuracy and reliability.

An **uncertainty analysis** is a process used to evaluate, characterise and propagate throughout a model the inherent uncertainties, variability and/ or imprecisions associated with LCSA data (Heijungs and Huijbregts, 2004). It enables a practitioner to eventually obtain a probabilistic range of impact results, instead of a single nominal score.

Sensitivity analysis and uncertainty analysis can be conducted jointly within the LCSA context. This is done by considering uncertainty the source of variability that is to be assessed by the sensitivity analysis. In this sense, a common practice is to first perform an uncertainty analysis to identify how the characterised uncertainties in the input data propagate throughout a model, to then complete a sensitivity analysis to determine how influential each of the factors subject to such uncertainties is.

Sensitivity analysis in LCSA

Example: (from SH2E deliverable D6.3, regarding the LCSA and benchmarking of a PEMFC passenger car)

“As previously mentioned, cases of multi-functionality were addressed through system expansion for SMR hydrogen production […] Three additional scenarios were created using energy, physical, and economic allocations to explore the effect of the approaches to multi-functionality through sensitivity analysis.”

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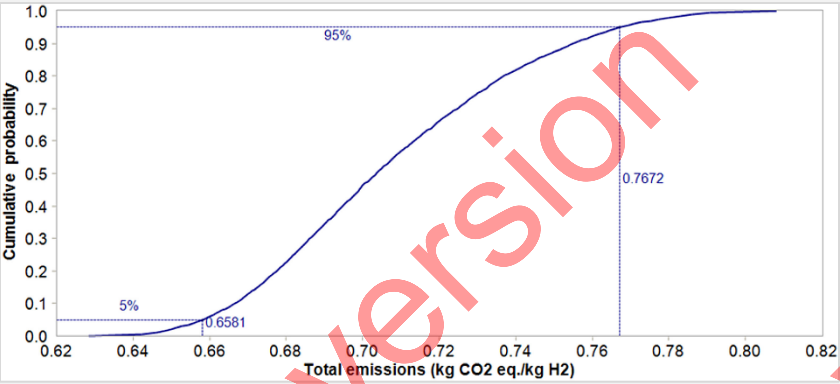
Uncertainty analysis in LCSA

Example: (from reference [Ghandehariun and Kumar, 2016], on the LCA of wind-based hydrogen production in Western Canada)

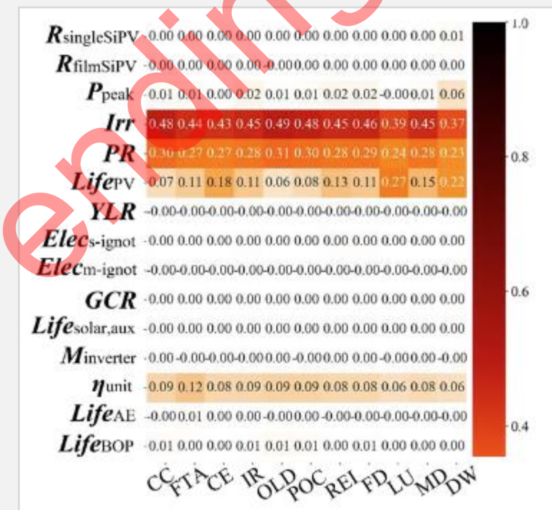
"An uncertainty analysis was performed by building a Monte Carlo simulation model through ModelRisk. Table 6 shows the variations in key input parameters. The results for the overall GHG emissions are presented in Fig. 4. As can be seen, with a 95% level of confidence, GHG emissions of the plant range between 0.66 and 0.77 kg CO_2 eq./kg H_2."



Uncertainty analysis together with sensitivity analysis in LCSA

Example: (from reference [Zhang et al., 2022], on uncertainty and sensitivity analysis on the environmental profile of hydrogen production in France)

"Figure 9a shows the first-order Sobol indices for each impact category and input parameter […] For each impact category studied, under French national average resource availability and technology mix 2019, around 38 %-50 % LCIA results' variability comes from the variation of French annual solar irradiation available on PV panels. About 23 %-30 % LCIA results variations come from the uncertainty of the PV panel performance ratio. The remaining LCIA results' variations mainly come from PV panel lifetime uncertainty".



(vertical axis: acronym for parameters; horizontal axis: acronym for the assessed impact categories)

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6.2 Integration

Interpreting LCSA results can prove challenging due to the diverse nature of individual findings. These results consist of various indicators measured in distinct unit. Accordingly, it is unfeasible to suggest one single unequivocal solution unless one alternative outperforms all others across all indicators. Identifying the optimal alternative, encompassing a spectrum of sustainability indicators, within a decision-making context, is a challenging task. It is necessary to not solely compare indicators within one assessment, e.g., LCA. It is also important to assess indicators across all three assessments, spanning LCA, LCC and SLCA.

To synthesise individual indicator results within LCSA, mathematical procedures are used. Initially, these procedures necessitate the assignment of weights to individual indicators. In this regard, **Multi-Criteria Decision Analysis (MCDA)** methods, designed to facilitate diverse decision-making processes, can provide invaluable assistance in interpreting LCSA results. MCDA encompasses a suite of mathematical approaches that condense a vast array of individual results into a more manageable subset, promoting a more nuanced understanding of the overarching sustainability picture (Prado et al., 2012; Jones, 2016).

Given the nascent stage of LCSA and the myriad uncertainties it entails, as well as the diverse objectives it seeks to address, the UNEP/SETAC recommends the presentation of raw results without applying weighting and aggregation (Valdivia et al., 2011). This approach allows for a nuanced exploration of the issues at hand, preserving the richness of information without oversimplification. However, there is a preference for generating results that are readily communicable, not only for practical use in policy and economics but also to foster productive scientific discourse (Finkbeiner et al., 2012). Furthermore, when **weighting and grouping** are not explicitly carried out, each reader inevitably imparts their own implicit weighting based on their individual value system, potentially leading to divergent interpretations (Wulf et al., 2019).

Figure 5 depicts an approach to integrating MCDA into an LCSA study. In addition to its various mathematical methods, MCDA centres on the integration of stakeholders. These stakeholders can be decision-makers in industry, politicians, citizens, etc. MCDA allows for the integration of these stakeholders into the entire decision-making process at numerous levels, including the goal and scope definition of an LCSA. More frequently, they are incorporated when determining the weighting factors for the diverse impact categories in an LCSA. In a thorough MCDA process, stakeholders must also be involved in interpreting the outcomes. Further explanation on normalisation, grouping and weighting is provided in the following sections. If MCDA methods are used, it is crucial to acknowledge that they rely on values that require cautious treatment by the practitioners.

Grouping

Various techniques can be used to group impact categories in LCSA. Typically, linear aggregation methods enable the full compensation of impact categories. One well-known technique is the weighted sum approach, also called simple additive weighting (Wulf et al., 2017). While easy to use, this method does not account for more complex decision-making contexts. The Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS) (Haase et al., 2020) is a more intricate MCDA approach that takes into consideration the compensation of impacts. TOPSIS smooths out some of the drawbacks of the weighted sum method. VIKOR (Hashemkhani Zolfani et al., 2020), which falls under the same category of methods, is also noteworthy. Prior to using any of these aggregation methods, normalisation is necessary.

If compensation between different impact categories and sustainability dimensions is not permitted by the practitioner, it is recommended to use outranking methods. The two most prominent ones are the Preference Ranking Organization METHod for Enrichment Evaluation (PROMETHEE) (Bahzadian et al., 2010) and Elimination Et Choix Traduisant la

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REalité (ELECTRE) (Figueira et al., 2005). More effort is required, such as defining thresholds for each impact category. While the results may be less transparent, they are also more robust.

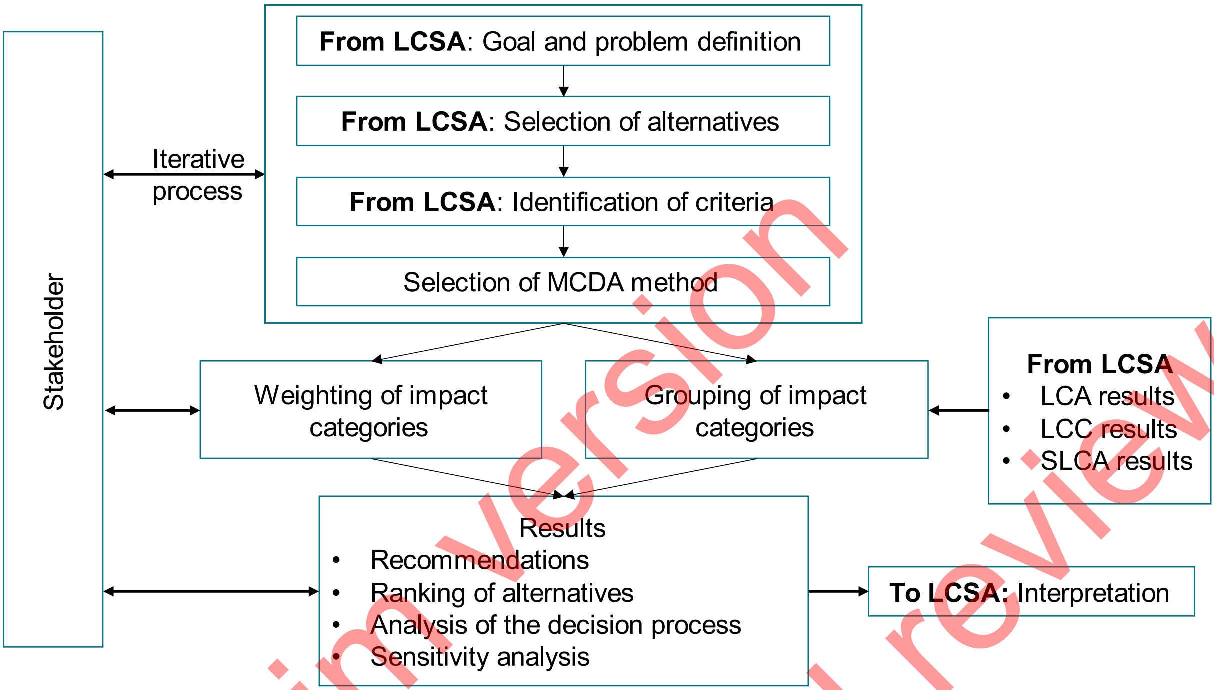

Figure 5. Generic approach to integrating MCDA into LCSA, based on Haase et al. (2021).

Normalisation

In general, there are two approaches to normalising data. One entails using internal statistical techniques, while the other involves cross-referencing against external benchmarks. Internal normalisation necessitates division with respect to the range between the minimum and maximum values (min-max or linear normalisation) or on a minimum, maximum, or benchmark basis. Other forms of internal normalisation include vector and logarithmic normalisation (Hashemkhani Zolfani et al., 2020). Internal normalisation by division is problematic due to the possibility, albeit rare, of the rank order of alternatives being reversed after aggregation. As a result, this method is highly controversial in LC(S)A and is mostly avoided by practitioners, who prefer external normalisation instead (Prado et al., 2012; Verones et al., 2016).

Another normalisation method is external reference points. These can encompass the global or local average impact category per person, or a political target value for this category (Prado et al., 2012; De Benedetto and Klemeš, 2009). The use of normalised results allows for the evaluation of the impact's significance within a global context, and the identification of relevant impacts. Such normalisation is frequently deployed in LC(S)A independently. The use of external normalisation factors can heighten uncertainty in the comprehensive evaluation owing to the intricacies of ascertaining reference factors, probable dearth or disparity of data, and the reality that some impact categories highlight regional rather than worldwide consequences. Consequently, reliance on global values for comparison may result in over- or underestimation of impacts (Prado et al., 2017).

The selection of the normalisation method can substantially impact the overall MCDA and, consequently, in turn the LCSA results (Hashemkhani Zolfani et al., 2020; Prado et al., 2017). Though these methods may receive lesser attention, they should be chosen with the same level of care as all other steps of an MCDA.

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Weighting

Various methods can be used to identify weighting factors with and without the integration of stakeholders. The most popular and straightforward approach is to use equal weights for all impact categories or with a hierarchical structure, where the first level are the three sustainability dimensions or assessment methods (OECD, 2008). Within each assessment, every indicator is assigned a weighting factor at the second hierarchical level. This can ensure results that are dependable and sturdy when coupled with a sensitivity analysis (Prado et al., 2012; Ibáñez-Forés et al., 2013). The impact of the hierarchical structure of the study on the overall outcome of the MCDA must be taken into account. Various studies have investigated alternative hierarchical structures, such as those aligned with the Sustainable Development Goals, and their effect on the results of the MCDA (Blok et al., 2013; Wulf et al., 2022b).

An alternative theoretical approach used in LCSA for determining weighting factors involves the stakeholder profiles of individualists, hierarchists, and egalitarians from cultural theory. As each stakeholder profile prioritises the sustainability dimensions differently, the application of the cardinal ranking method yields distinct weighting factors (Ekener et al., 2018).

In certain decision-making contexts, it may be preferable to involve representative stakeholders in order to promote a participatory and collaborative decision-making process. This necessitates the implementation of an interface whereby stakeholders can communicate their preferences with regard to the chosen criteria. Moreover, MCDA techniques can identify diverging opinions and facilitate resolving potential discrepancies (Goodwin and Wright, 2014). Various methods can engage participants, such as interviews, decision conferencing or online surveys (Marttunen et al., 2015). The choice of method depends on factors such as the number of stakeholders, resource availability, and complexity of the issue. Various methods are available for assigning weightings, such as those based on trade-offs (Simple Multi Attribute Rating Technique, SMART), direct ratings, lotteries, and pairwise comparisons, for example, the Analytic Hierarchy Process (AHP) (Saaty, 1977). While SMART and AHP offer means of defining weightings that are universally applicable, other methods, such as conjoint analysis and the discrete choice experiment, are dependent on their specific use cases (Tarne et al., 2019).

For Environmental Footprint calculations, Sala et al. (2018) developed a universal weighting factor set including all impact categories. Surveys were conducted among various stakeholder groups, including lay people, LCA experts, and a workshop with Life Cycle Impact Assessment experts. The results were subsequently combined with a robustness factor for each environmental indicator. However, as similar weighting factors are missing for LCC and SLCA, it is difficult to incorporate them into LCSA.

It should be noted that surveys and interviews have restricted applicability and transferability of findings due to their temporal and geographic limitations, as well as the possibility of being specific to a particular case study.

6.3 Reporting

One additional aspect to note in interpretation is the visual display of results, which can support the identification of significant contributions as well as of inconsistencies. There are already tools such as the Life Cycle Sustainability Dashboard (Traverso et al., 2012), Sustainability Crowns (Corona and San Miguel, 2019), and Life Cycle Sustainability Triangle (Finkbeiner et al., 2010). However, each of the aforementioned methods comes with its own limitations (Backes et al., 2023) that should be realised prior to use. Learnt lessons from these tools can be:

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- A dashboard-like overview is useful, as it helps users get the full picture before going in more detail.
- A full drill-down is helpful to understand contributions and also identify potential inconsistencies.
- A combination of different visualisations (in the simplest form, as multi-scatter plot) helps practitioners detect inconsistencies and relations.
- A grouping and classification of “similar things” is often helpful; this can be implemented in the form of a cluster analysis dendrogram, or similar.

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REFERENCES

Arvidsson R, Tillman AM, Sandén BA, Janssen M, Nordelöf A, Kushnir D, et al. Environmental Assessment of Emerging Technologies: Recommendations for Prospective LCA. J Ind Ecol. 2018; 22(6):1286–1294.

Backes JG, Traverso M. Life cycle sustainability assessment as a metrics towards SDGs agenda 2030. Curr Opin Green Sustain Chem. 2022; 38:100683. https://doi.org/10.1016/j.cogsc.2022.100683

Backes J, Steinberg L, Weniger A, Traverso M. Visualization and Interpretation of Life Cycle Sustainability Assessment—Existing Tools and Future Development. Sustainability. 2023; 15(13):10658. https://doi.org/10.3390/su151310658

Bargiacchi E, Puig-Samper G, Campos-Carriedo F, Iribarren D, Dufour J, Ciroth A, et al. D2.2 Definition of FCH-LCA guidelines. 2022.

Bauman H, Tillman A-M. The Hitch Hiker's Guide to LCA. Studentlitteratur AB; 2004.

Bean L, Thomas DW. Development of the judicial definition of materiality. Accounting Historians Journal. 1990; 17:2.

Blok K, Huijbregts M, Patel M, Hertwich E, Hauschild M, Sellke P, et al. Handbook on a Novel Methodology for the Sustainability Impact Assessment of New Technologies. Utrecht: Utrecht University; 2013.

Behzadian M, Kazemzadeh RB, Albadvi A, Aghdasi M. PROMETHEE: A comprehensive literature review on methodologies and applications. European Journal of Operational Research. 2010;200:198-215.

Bouillass G, Blanc I, Perez-Lopez P. Step-by-step social life cycle assessment framework: a participatory approach for the identification and prioritization of impact subcategories applied to mobility scenarios The International Journal of Life Cycle Assessment. 2021;26, 2408–2435. https://doi.org/10.1007/s11367-021-01988-w

Ciroth A. Uncertainties in life cycle assessment. Int J Life Cycle Assess. 2004; 9(3):141–142. https://doi.org/10.1007/BF02994186

Ciroth, A. Validation – The Missing Link in Life Cycle Assessment. Towards pragmatic LCAs. Int J Life Cycle Assess. 2006; 11:295–297. https://doi.org/10.1065/lca2006.09.271

Ciroth A, Barreiros T, Cortés D, Puig-Samper, Gonzalo Bargiacchi E, Iribarren D, Dufour J. D2.1 Review on LCA guidelines and LCA of FCH systems. 2021.

Corona B, San Miguel, G., Life cycle sustainability analysis applied to an innovative configuration of concentrated solar power. Int J Life Cycle Assess. 2019; 24:1444–1460. https://doi.org/10.1007/s11367-018-1568-z

Costa D, Quinteiro P, Dias AC. A systematic review of life cycle sustainability assessment: Current state, methodological challenges, and implementation issues. Sci Total Environ. 2019; 686:774–787. https://doi.org/10.1016/j.scitotenv.2019.05.435

De Benedetto L, Klemeš J. The Environmental Performance Strategy Map: an integrated LCA approach to support the strategic decision-making process. J Clean Prod. 2009; 17:900–906.

Ekener E, Hansson J, Larsson A, Peck P. Developing Life Cycle Sustainability Assessment methodology by applying values-based sustainability weighting - Tested on biomass based and fossil transportation fuels. Journal of Cleaner Production. 2018; 181:337–351.

European Commission. Joint Research Centre. Institute for Environment and Sustainability. International Reference Life Cycle Data System (ILCD) Handbook general guide for life cycle assessment: detailed guidance. Publications Office; 2010.

This project has received funding from the Fuel Cells and Hydrogen 2 Joint Undertaking (now Clean Hydrogen Partnership) under Grant Agreement No 101007163. This Joint Undertaking receives support from the European Union's Horizon 2020 Research and Innovation program, Hydrogen Europe and Hydrogen Europe Research.

European Commission. Recommendation 2013/179/EU on the use of common methods to measure and communicate the life cycle environmental performance of products and organisations. Off J Eur Union. 2013; (L 124):210.

European Union. Directive (EU) 2022/2464 of the European Parliament and of the Council of 14 December 2022. Strasbourg, France: 2022.

Figueira J, Mousseau V, Roy B. Electre Methods. In: Figueira J, Greco S, Ehrogott M, editors. Multiple Criteria Decision Analysis: State of the Art Surveys. New York, NY: Springer New York; 2005. p. 133–153.

Finkbeiner M, Schau EM, Lehmann A, Traverso M. Towards Life Cycle Sustainability Assessment. Sustainability. 2010; 2(10):3309–3322.

Funtowicz SO., Ravetz, JR. Uncertainty and quality in science for policy. (W. Leinfellner, Ed.). Dordrecht: Kluwer Acadmic Publishers; 1990. http://doi.org/10.1007/978-94-009-0621-1

Ghandehariun S, Kumar A. Life cycle assessment of wind-based hydrogen production in Western Canada. Int J Hydrogen Energy. 2016; 41(22):9696–9704. https://doi.org/10.1016/j.ijhydene.2016.04.077

Goodwin P, Wright G. Decision Analysis for Management Judgment. 5th ed. Hoboken: Wiley; 2014.

Greco, S., Ishizaka, A., Tasiou, M. Torrisi, G. On the Methodological Framework of Composite Indices: A Review of the Issues of Weighting, Aggregation, and Robustness. Soc Indic Res. 2019; 141:61–94. https://doi.org/10.1007/s11205-017-1832-9

GRI. The GRI Perspective. The materiality madness: why definitions matter. Amsterdam; 2022.

GRI. GRI 3: Material Topics 2021. Amsterdam; 2023a.

GRI. Resource center. https://www.globalreporting.org/how-to-use-the-gri-standards/resource-center/; 2023b [13.10.2023].

GRI. GRI 11: Oil and Gas Sector 2021. Amsterdam; 2023c.

Guinee JB, Lindeijer E. Part 3: Scientific background. In Handbook on life cycle assessment: operational guide to the ISO standards. In: An operational guide to the ISO-standards. Springer Science & Business Media; 2002.

Haase M, Babenhauserheide N, Rösch C. Multi criteria decision analysis for sustainability assessment of 2nd generation biofuels. Procedia CIRP. 2020; 90:226–231.

Haase M, Baumann M, Wulf C, Rösch C, Zapp P. Multikriterielle Analysen zur Entscheidungsunterstützung in der Technikfolgenabschätzung. In: Böschen S, Grunwald A, Krings B-JMA, Rösch C, editors. Technikfolgenabschätzung: Handbuch für Wissenschaft und Praxis. 1 ed. Baden-Baden: Nomos Verlagsgesellschaft mbH & Co. KG; 2021. p. 306–320.

Hashemkhani Zolfani S, Yazdani M, Pamucar D, Zarate P. A VIKOR and TOPSIS focused Reanalysis of the MADM Methods based on Logarithmic Normalization. Facta Universitatis, Series: Mechanical Engineering. 2020; 18:341–355.

Heijungs R, Huijbregts MAJ. A Review of Approaches to Treat Uncertainty in LCA. In 2nd International Congress on Environmental Modelling and Software, Osnabrück, Germany, June 2004.

Ibáñez-Forés V, Bovea MD, Azapagic A. Assessing the sustainability of Best Available Techniques (BAT): methodology and application in the ceramic tiles industry. J Clean Prod. 2013; 51:162–176.

International Organization for Standardization. ISO 14040:2006 Environmental Management — Life cycle assessment —Principles and framework. Geneva, Switzerland; 2006a.

International Organization for Standardization. ISO 14044:2006 Environmental Management — Life cycle assessment — Requirements and guidelines. Geneva; 2006b.

This project has received funding from the Fuel Cells and Hydrogen 2 Joint Undertaking (now Clean Hydrogen Partnership) under Grant Agreement No 101007163. This Joint Undertaking receives support from the European Union's Horizon 2020 Research and Innovation program, Hydrogen Europe and Hydrogen Europe Research.

Iribarren D, Calvo-Serrano R, Martín-Gamboa M, Galán-Martín Á, Guillén-Gosálbez G. Social life cycle assessment of green methanol and benchmarking against conventional fossil methanol. Sci. Total Environ. 2022; 824:153840. https://doi.org/10.1016/j.scitotenv.2022.153840

Iribarren D, Campos-Carriedo F, Dufour J, di Noi C, Ciroth A, Murali SH, et al. D4.2 Definition of FCH-SLCA guidelines. 2023.

Jones M. Multi-Criteria Decision Analysis Tool. MEASURE. Manchester: The University of Manchester; 2016.

Klöpffer W, Grahl B. Life Cycle Assessment (LCA): A Guide to Best Practice. John Wiley & Sons; 2014.

Lotrič A, Sekavčnik M, Kuštrin I, Mori M. Life-cycle assessment of hydrogen technologies with the focus on EU critical raw materials and end-of-life strategies. Int J Hydrogen Energy. 2021; 46(16): 10143–10160. https://doi.org/10.1016/j.ijhydene.2020.06.190

Lozanovski A, Schuller O, Faltenbacher M. FC-HyGuide. Guidance Document for Performing LCA on Hydrogen Production Systems. 2011.

Marttunen M, Mustajoki J, Dufva M, Karjalainen TP. How to design and realize participation of stakeholders in MCDA processes? A framework for selecting an appropriate approach. EURO Journal on Decision Processes. 2015;3 :187-214.

Masoni P, Zamagni A. FC-HyGuide. Guidance Document for performing LCAs on Fuel Cells. Brussels, Belgium; 2011.

OECD. Handbook on constructing composite indicators methodology and user guide. Paris: OECD; 2008.

OECD. OECD due diligence guidance for responsible business conduct. Paris: OECD; 2018.

OECD. Responsible business conduct. OECD Guidelines for Multinational Enterprises. https://mneguidelines.oecd.org//sectors/; 2023 [17.10.2023].

Ortigueira J, Pacheco M, Trancoso MA, Farrancha P, Correia J, Silva C, et al. Food waste biorefinery: Stability of an acidogenic fermentation system with carbon dioxide sequestration and electricity generation. J. Clean. Prod. 2020; 270:122040. https://doi.org/10.1016/j.jclepro.2020.122040

Pihkola H, Cordella M, Behm K, Horn R, Zamagni A, Zanchi L, et al. D2.3 LCSA methodology to be implemented in WP4 demonstrations WP2 LCSA methodology. 2022.

Prado V, Rogers K, Seager TP. Integration of MCDA Tools in Valuation of Comparative Life Cycle Assessment. In: Curran MA, editor. Life cycle assessment handbook a guide for environmentally sustainable products. Hoboken: Wiley; 2012. p. 413–432.

Prado V, Wender BA, Seager TP. Interpretation of comparative LCAs: external normalization and a method of mutual differences. The International Journal of Life Cycle Assessment. 2017; 22:2018–2029.

Puig-Samper G, Bargiacchi E, Iribarren D, Dufour J. Assessing the prospective environmental performance of hydrogen from high-temperature electrolysis coupled with concentrated solar power. Renew Energy. 2022; 96:1258–1268. https://doi.org/10.1016/J.RENENE.2022.07.066.

Saaty TL. A scaling method for priorities in hierarchical structures. Journal of Mathematical Psychology. 1977;15:234–281.

Sala S, Cerutti AK, Pant R. Development of a weighting approach for the Environmental Footprint. Luxembourg: Publications Office of the European Union; 2018.

Sousa-Zomer TT, Cauchick Miguel PA. The main challenges for social life cycle assessment (SLCA) to support the social impacts analysis of product-service systems. Int J Life Cycle Assess. 2018; 23:607–616. https://doi.org/10.1007/s11367-015-1010-8

This project has received funding from the Fuel Cells and Hydrogen 2 Joint Undertaking (now Clean Hydrogen Partnership) under Grant Agreement No 101007163. This Joint Undertaking receives support from the European Union's Horizon 2020 Research and Innovation program, Hydrogen Europe and Hydrogen Europe Research.

Susmozas A, Iribarren D, Dufour J. Life-cycle performance of indirect biomass gasification as a green alternative to steam methane reforming for hydrogen production. Int J Hydrogen Energy. 2013; 38(24):9961–9972. https://doi.org/10.1016/j.ijhydene.2019.01.105

Swarr TE, Hunkeler D, Klöpffer W, Pesonen H-L, Ciroth A, Brent AC, et al. Environmental life cycle costing: A code of practice. Pensacola. Brussels: SETAC; 2011.

Tarne P, Lehmann A, Finkbeiner M. Introducing weights to life cycle sustainability assessment—how do decision-makers weight sustainability dimensions? The International Journal of Life Cycle Assessment. 2019;24:530–542.

Tragnone BM, D'Eusanio M, Petti L. The count of what counts in the agri-food Social Life Cycle Assessment. Journal of Cleaner Production. 2022; 354:131624. https://doi.org/10.1016/j.jclepro.2022.131624

Traverso M, Finkbeiner M, Jørgensen A, Schneider L. Life cycle sustainability dashboard. J Ind Ecol. 2012; 16(5):680-688. https://doi.org/10.1111/j.1530-9290.2012.00497.x

UNEP. Guidelines for Providing Product Sustainability Information. Global guidance on making effective environmental, social and economic claims, to empower and enable consumer choice. 2017. Retrieved from: https://wedocs.unep.org/20.500.11822/22180

UNEP. Guidelines for Social Life Cycle Assessment of Products and Organizations 2020. 2020. Retrieved from http://www.unep.fr/shared/publications/pdf/DTIx1164xPA-guidelines_sLCA.pdf

Valdivia S, Ugaya CML, Sonnemann G, Hildebrand J, Ciroth A, Finkbeiner M, et al. Towards a Life Cycle Sustainability Assessment: Making informed choices on products. Paris: UNEP/SETAC Life Cycle Initiative; 2011.

Valdivia S, Backes JG, Traverso M, Sonneman, G, Cucurachi S, Guinée JB, et al. Principles for the application of life cycle sustainability assessment. Int J Life Cycle Assess. 2021;26:1900–1905. https://doi.org/10.1007/s11367-021-01958-2

Valente A, Iribarren D, Candelaresi D, Spazzafumo G, Dufour J. Using harmonised life-cycle indicators to explore the role of hydrogen in the environmental performance of fuel cell electric vehicles. Int J Hydrogen Energy. 2020; 45(47):25758–25765. https://doi.org/10.1016/j.ijhydene.2019.09.059

Valente A, Iribarren D, Dufour J. Comparative life cycle sustainability assessment of renewable and conventional hydrogen. Sci Total Environ. 2021; 756:144132. https://doi.org/10.1016/j.scitotenv.2020.144132

Van der Giesen C, Cucurachi S, Guinée J, Kramer GJ, Tukker A. A critical view on the current application of LCA for new technologies and recommendations for improved practice. J Clean Prod. 2020; 259:120904. https://doi.org/10.1016/j.jclepro.2020.120904

Verones F, Henderson A, Laurent A, Ridoutt B, Ugaya C, Hellweg S. LCIA framework and modelling guidance [TF 1 Crosscutting issues]. In: Frischknecht R, Jolliet O, editors. Global Guidance for Life Cycle Impact Assessment Indicators. Paris: UNEP DTIE Sustainable Lifestyles, Cities and Industry Branch; 2016.

Wei, W., Larrey-Lassalle, P., Faure, T., Dumoulin, N., Roux, P., & Mathias, J.-D. How to Conduct a Proper Sensitivity Analysis in Life Cycle Assessment: Taking into Account Correlations within LCI Data and Interactions within the LCA Calculation Model. Environ. Sci. Technol. 2015; 49(1), 377–385. https://doi.org/10.1021/es502128k

Wulf C, Zapp P, Schreiber A, Marx J, Schlör H. Lessons Learned from a Life Cycle Sustainability Assessment of Rare Earth Permanent Magnets. Industrial Ecology. 2017; 21:1578–1590.

Wulf C, Werker J, Ball C, Zapp P, Kuckshinrichs W. Review of Sustainability Assessment Approaches Based on Life Cycles. Sustainability. 2019; 11:5717.

This project has received funding from the Fuel Cells and Hydrogen 2 Joint Undertaking (now Clean Hydrogen Partnership) under Grant Agreement No 101007163. This Joint Undertaking receives support from the European Union's Horizon 2020 Research and Innovation program, Hydrogen Europe and Hydrogen Europe Research.

Wulf C, Zapp P, Schonhoff A, Bargiacchi E, Iribarren D, Dufour J, et al. D4.1 Definition of FCH-LCC guidelines WP4 Harmonised extension to Life Cycle costing and Social Life Cycle Assessment. 2022a.

Wulf C, Zapp P, Schreiber A, Kuckshinrichs W. Integrated Life Cycle Sustainability Assessment: Hydrogen Production as a Showcase for an Emerging Methodology. In: Klos ZS, Kalkowska J, Kasprzak J, editors. Towards a Sustainable Future - Life Cycle Management: Challenges and Prospects. Cham: Springer International Publishing; 2022b. p. 97–106.

Wulf C, Haase M, Baumann M, Zapp P. Weighting factor elicitation for sustainability assessment of energy technologies. Sust Energy Fuels. 2023; 7(3):832–847. https://doi.org/10.1039/D2SE01170K.

Zapp P, Schreiber A. SH2E D3.1 Material criticality indicator. Brussels: Clean Hydrogen Partnership; 2021.

Zhang Z, Douziech M, Pérez-López P, Wang Q, Yang Q. Identify Parameters Hindering Renewable Hydrogen Production in France: Life Cycle Sensitivity and Uncertainty Analysis. E3S Web of Conferences 2022; 350:01021. https://doi.org/10.1051/e3sconf/202235001021

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ANNEX 1 - LIFE CYCLE ASSESSMENT OF POWER-TO-SYNGAS: COMPARING HIGH-TEMPERATURE CO-ELECTROLYSIS AND STEAM METHANE REFORMING

1. GOAL OF THE LIFE CYCLE ASSESSMENT

The **goal** of this LCA study is to evaluate the environmental profile of syngas production by high-temperature co-electrolysis (HT-Co-EC) coupled with direct air capture (DAC) in 2030, and benchmark it to that of conventional syngas from a small-scale steam methane reformer. Steam methane reforming (SMR) is the standard technology for syngas production.

Although the progressive implementation of new (renewable) syngas pathways is expected to have a large scale-effect, this study places the focus on accounting for the potential environmental impacts of the specific syngas product, with decision-support limited to the specific product (i.e. micro-level decision support). A **prospective attributional** life cycle inventory (LCI) modelling approach was chosen. The present LCA study is not meant for decision making at meso or macro level, as it aims at defining the prospective environmental profile of syngas from HT-Co-EC and comparing it to that of conventional syngas production by SMR. Moreover, this study should be understood as case-specific.

2. SCOPE OF THE LIFE CYCLE ASSESSMENT

2.1 Modelling approach

The current LCA study places the focus on defining the environmental profile of syngas produced by HT-Co-EC coupled with DAC. As the technology readiness level (TRL) of this type of electrolysis is around 5, expecting to reach full maturity by 2030, the system was modelled based on the year 2030 to appropriately explore the potential of this syngas option. In this sense, the present LCA was approached from a **prospective point of view**.

2.2 Prospectivity

The system under evaluation was modelled based on the **year 2030**, when HT-Co-EC technology is expected to reach full technical maturity. Thus, the HT-Co-EC part of the system was modelled according to the expected technical performance indicators for 2030 (e.g. efficiency and cell degradation rate). The modelling of HT-Co-EC operation and the benchmark syngas production by small-scale SMR were based on Aspen process simulation. External electricity demand linked to the foreground system involved a prospective electricity mix for 2030. Data of the DAC plant represent the existing Climeworks DAC plant in Hinwil. General assumptions about a possible reduction in energy demand by 40% in the future were not considered here, but can be introduced through a sensitivity analysis.

2.3 Functional unit

The only function of the system is to produce syngas. Hence, only one functional flow was involved. The **functional unit** (FU) of the study was defined as the production of 1 kg of syngas with a molar hydrogen-to-CO ratio of two ($H_2/CO=2$), at 20 bar, 40 °C and a carbon dioxide molar fraction below 0.1 mol%. Although syngas and oxygen are produced during the HT-Co-EC, no allocation was carried out between the two products. Oxygen is neither purified, nor stored or used. Before the oxygen is released from the system, it is diluted with air to mitigate safety concerns. Therefore, it was considered as waste and no allocation was deemed necessary.

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The FU of the competing system for benchmarking (syngas from fossil based small-scale SMR) was also defined as 1 kg of syngas at the same above-mentioned conditions.

2.4 System boundaries

The system boundaries of the study follow a **cradle-to-gate perspective**, encompassing all life-cycle phases of the system under evaluation from raw material extraction to syngas production (Figure 1-A1). The production system involves two main sections: (i) the syngas production unit, and (ii) the DAC plant. All auxiliary energy and material flows entering or leaving these sections were considered. The process design derived a fully heat-integrated process, so that no steam input and export was required neither for the HT-Co-EL nor for the SMR. To achieve the desired hydrogen-to-CO ratio of two not only the HT-Co-EL needs external carbon monoxide from the DAC but also the SMR. Processing and use of syngas for a specific industrial application was left out of the presented scope. Decommissioning of the production units or other end-of life processes were neglected. No cut-off was applied.

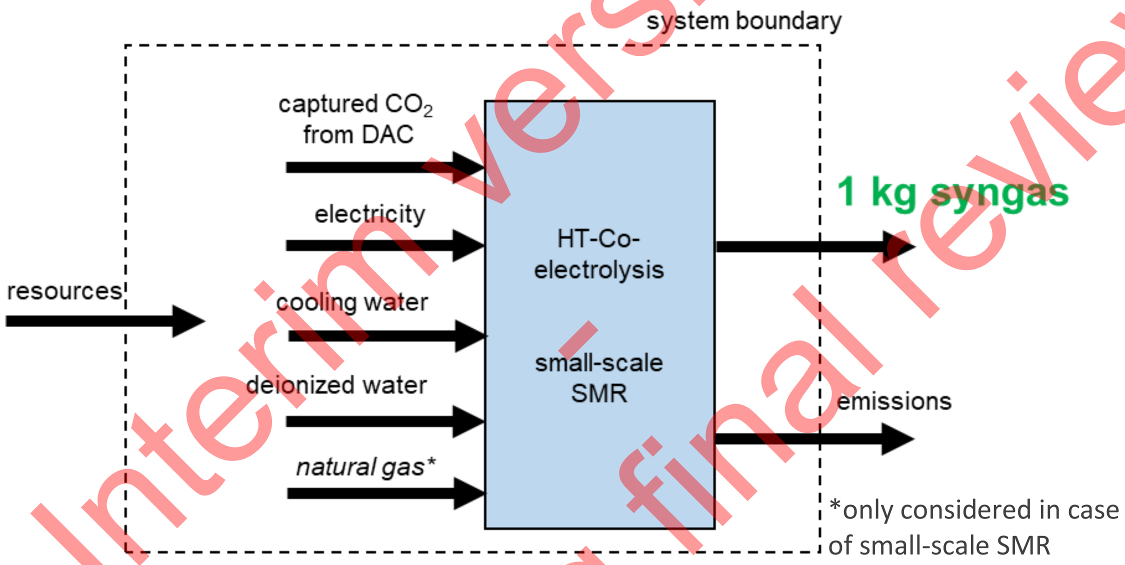

Figure 1-A1. System boundary of the LCA for syngas production (DAC: Direct Air Capture, HT: High-Temperature; SMR: Steam Methane Reforming).

Capital goods (without EoL) directly relevant to the entire foreground system under evaluation (HT-Co-EC system including cells, stack, balance of plant [BoP]; DAC system; small-scale steam methane reformer) were included in this analysis. The lifetime of the small-scale steam methane reformer, DAC system and HT-Co-EC system was assumed to be 20 years except for the HT-Co-EC stacks and cells (ten years). Capital goods belonging to the background processes (e.g. supply of deionised water, electricity, natural gas) were considered relying on the information provided by the selected background database (ecoinvent v.3.8, Sphera database v. 10.7.0.183).

2.5 Multi-functionality

There is no multi-functionality neither with the SMR nor with the HT-Co-EC due to the heat integration scheme in the system design.

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3. LIFE CYCLE INVENTORY

The LCI corresponding to the modelling of the **foreground system** was retrieved from a work previously developed within the context of the German Kopernikus project (Schreiber et al., 2020). Both syngas production plants operate at maximum full load hours (8760 h).

3.1 Data sources and availability

Most of the LCI data of the syngas production technologies (foreground data) were provided by Kopernikus project partners:

1. Cell and stack construction of HT-Co-EC:
   - Forschungszentrum Jülich GmbH – Institute of Energy and Climate Research (IEK-1, IEK-3).
   - Forschungszentrum Jülich GmbH – Central Institute of Engineering, Electronics and Analytics (ZEA).
2. Small-scale SMR process design and simulation, HT-Co-EC overall system design and process simulation:
   - Linde Aktiengesellschaft (AG), Linde Engineering, Research & Development, Process Development.
3. DAC:
   - Climeworks AG.
4. Electricity supply models:
   - Technical University Munich – Institute for Renewable and Sustainable Energy Systems.

For the **background processes** (e.g. electricity and water supply), the ecoinvent 3.8 database (system model "Allocation, cut-off by classification") was used. The complete LCI of the foreground and background system is provided in Schreiber et al. (2020).

A simplified electricity supply scenario for 2030 was assumed (Table 1-A1) according to a climate protection target of 80% carbon dioxide reduction compared to 1990, which supplies electricity to both syngas production plants.

Table 1-A1. Simplified Germany electricity supply mix 2030 based on Bareiß et al. (2018, 2019).

Energy technology	Ecoinvent 3.8 process	Share in electricity mix
Natural gas power plant	DE: electricity production, natural gas, combined cycle power plant	17%
Wind energy	DE: electricity production, wind, >3MW turbine, onshore	43%
Photovoltaic	DE: electricity production, photovoltaic, 570kWp open ground installation, multi-Si	24%
Lignite power plant	DE: electricity production, lignite	6%
Hard coal power plant	DE: electricity production, hard coal	10%

4. LIFE CYCLE IMPACT ASSESSMENT

The Life Cycle Impact Assessment (LCIA) method package selected for the study was the **Environmental Footprint version 3.1**, published by the Joint Research Centre (JRC). Table 2-A1 provides an overview of the midpoint environmental impact categories and indicators included in EF 3.1, their reference units, and the corresponding results of the two syngas

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production systems related to 1 kg of syngas produced (FU). Figure 2-A1 shows a graphic representation of the results. Overall, the electricity supply generally dominates the environmental performance of the HT-Co-EC system (Figure 3-A1). In case of syngas production by small-scale SMR, the additional supply of natural gas is significant. No normalisation, grouping or weighting of impact categories was performed.

Table 2-A1. LCIA results to produce 1 kg syngas according to the EF3.1 method package in 2030.

Impact categories and indicators	Reference Unit	HT-Co-EC	Small-scale SMR
Acidification	mol H^+ eq	3.73E-03	1.16E-03
Climate change	kg CO_2 eq	2.99E+00	1.56E+00
Climate change – Biogenic	kg CO_2 eq	1.44E-03	4.13E-03
Climate change – Fossil	kg CO_2 eq	2.99E+00	1.56E+00
Climate change – Land use and LU change	kg CO_2 eq	1.12E-03	1.56E-04
Ecotoxicity, freshwater	CTUe	8.97E+00	6.86E-01
Ecotoxicity, freshwater - inorganics	CTUe	8.78E+00	6.70E-01
Ecotoxicity, freshwater - organics	CTUe	1.86E-01	1.59E-02
Energy resources: non-renewable	MJ net calorific value	4.39E+01	4.55E+01
Eutrophication, freshwater	kg P eq	2.44E-03	1.04E-04
Eutrophication, marine	kg N eq	2.02E-03	4.69E-04
Eutrophication, terrestrial	mol N eq	1.71E-02	4.92E-03
Human toxicity, cancer	CTUh	1.60E-09	2.60E-10
Human toxicity, cancer – inorganics	CTUh	1.10E-09	1.99E-10
Human toxicity, cancer – organics	CTUh	5.09E-10	6.07E-11
Human toxicity, non-cancer	CTUh	4.28E-08	1.75E-08
Human toxicity, non-cancer – inorganics	CTUh	4.14E-08	1.73E-08
Human toxicity, non-cancer – organics	CTUh	1.40E-09	2.45E-10
Ionising radiation	kBq U-235 eq	4.78E-02	4.21E-03
Land use	-	3.77E+01	1.73E+00
Ozone depletion	kg CFC11 eq	1.08E-06	2.25E-07
Particulate matter	disease inc.	4.09E-08	8.49E-09
Photochemical ozone formation	kg NMVOC eq	5.14E-03	1.41E-03
Material resources: metals/minerals	kg Sb eq	4.37E-05	2.06E-06
Water use	m^3 depriv.	6.42E-01	4.64E-02

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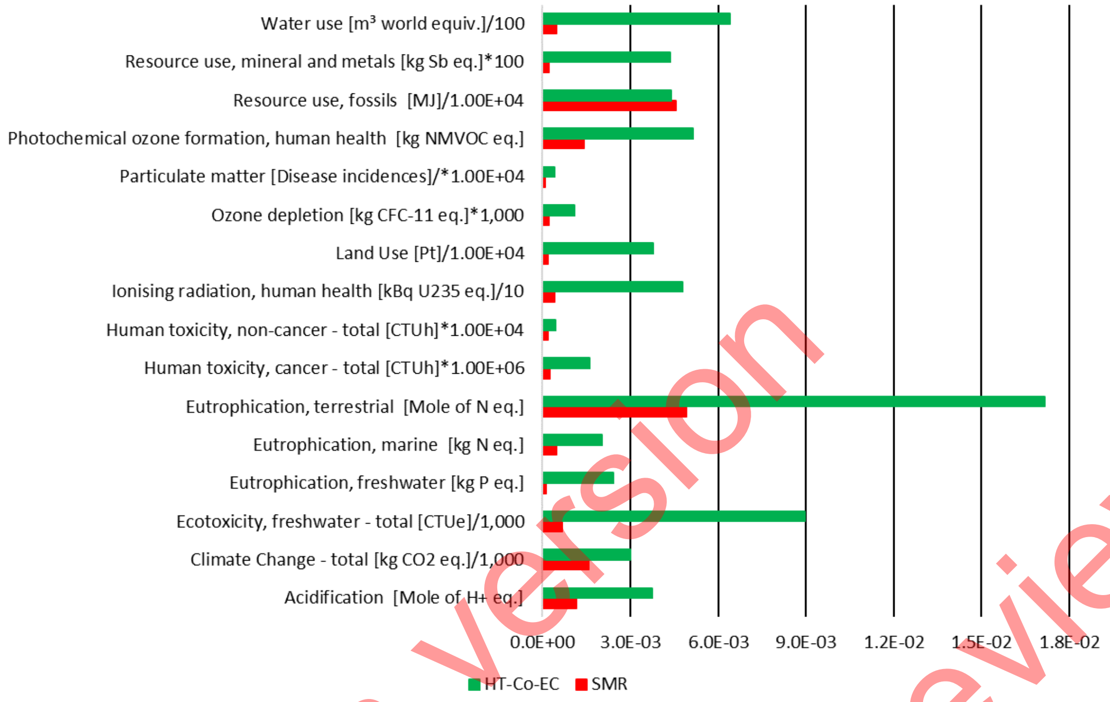

Figure 2-A1. Selected environmental impacts of 1 kg of syngas produced by HT-Co-EC and small-scale SMR.

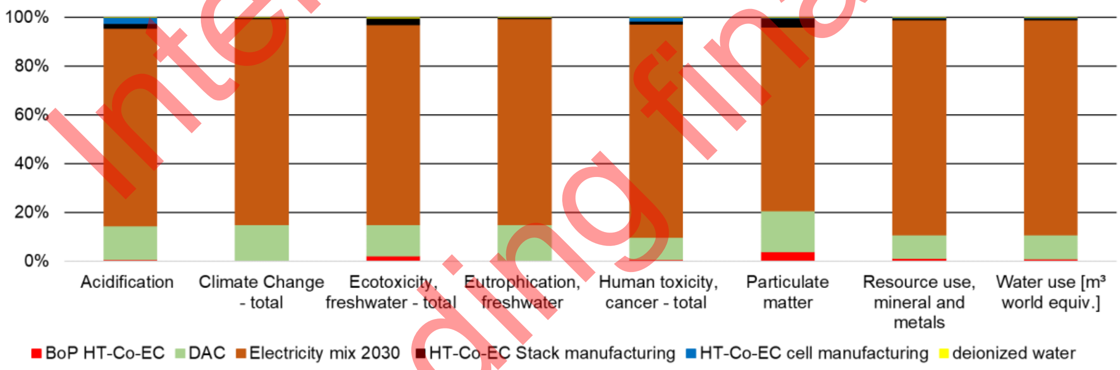

Figure 3-A1. Share of process chain segments of environmental impacts of 1 kg of syngas produced by HT-Co-EC.

5. INTERPRETATION AND FINAL REMARKS

The interpretation of this study includes the **benchmarking** of the prospective environmental profile of syngas production from HT-Co-EC against that of conventional syngas from SMR. Syngas production via SMR was selected as the benchmark system because it currently dominates the market (Rostrup-Nielson, 2005). For a meaningful comparison, only a small-scale steam methane reformer with an output of 330 m^3/h syngas was used as fossil reference. The SMR benchmark system was modelled under the same requirements, recommendations and methodological choices applied to the HT-Co-EC system, using the process simulation tool Aspen to build the full inventory.

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Conventional syngas from small-scale SMR was found to outperform syngas from HT-Co-EC in 15 out of the 16 environmental indicators shown in Table 2-A1 and Figure 2-A1. However, it should be highlighted that syngas from HT-Co-EC has a much more favourable carbon footprint if full-load hours are reduced or the share of renewable generation is increased (Figure 4-A1).

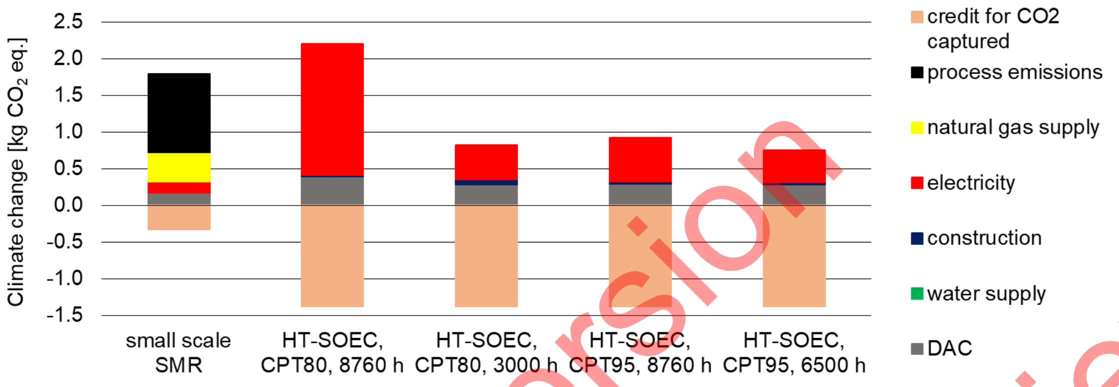

Figure 4-A1. Share of process stages on the total impact on Climate Change of 1 kg of syngas produced by small-scale SMR and HT-Co-EC supplied by different electricity mixes with different climate protection targets (CPT) and different full-load hours.

Overall, these results point out the future potential of HT-Co-EC and highlight the need for further research and technical development to ensure no burden-shifting across environmental impact categories.

6. REFERENCES

Bareiß K, Schönleber K, Hamacher T. Szenarien für den Strommix zukünftiger, flexibler Verbraucher am Beispiel von P2X-Technologien Technische Universität München, Lehrstuhl für Erneuerbare und Nachhaltige Energiesysteme; 2018.

Bareiß K, Schönleber K, Hamacher T. Erweiterung des bestehenden Technical Report „Szenarien für den Strommix zukünftiger, flexibler Verbraucher am Beispiel von P2X-Technologien" um das KSZ 55. Technische Universität München, Lehrstuhl für Erneuerbare und Nachhaltige Energiesysteme; 2019.

Rostrup-Nielson JR. Natural Gas: Fuel or Feedstock? . In: Derouane EG, Parmon V, Lemos F, Ribeiro FR, editors. Sustainable Strategies for the Upgrading of Natural Gas: Fundamentals, Challenges, and Opportunities Proceedings of the NATO Advanced Study Institute, held in Vilamoura, Portugal, July 6 - 18, 2003. Dordrecht, Netherlands: Springer Netherlands; 2005.

Schreiber A, Peschel A, Hentschel B, Zapp P. Life Cycle Assessment of Power-to-Syngas: Comparing High Temperature Co-Electrolysis and Steam Methane Reforming. Frontiers in Energy Research. 2020;8.

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ANNEX 2 - COMPLEMENTING A PROSPECTIVE LCA BY USING A PROSPECTIVE BACKGROUND DATABASE

When conducting an LCA study of an emerging technology, beyond the requirement of placing the foreground system at a future time by modelling its technical/operating parameters and capital goods in a prospective way, it is also recommended to use a **prospective database for background processes** (Boxes 4 and 5 of the present guidelines). By doing so, a better insight into the expected future performance of the system could be obtained, as the time-dependent economic and/ or industrial context in which such system would operate is integrated into the analysis. For instance, the consideration of a decarbonised electricity production mix might have an effect not only on the direct operation of a certain technology, but also on the upstream manufacturing processes alongside its supply chain.

In this sense, *premise* (2023) provides a consolidated framework to generate prospective scenarios of ecoinvent databases. It does so by merging the output results of Integrated Assessment Models (IAMs) such as REMIND or IMAGE into the original ecoinvent structure, generating completely equivalent databases in terms of operationalisation, which can be easily implemented in common LCA environments. For further information on *premise* and IAMs (i.e. approaches that integrate knowledge from two or more domains into a single framework, typically linking features of society and economy with the biosphere and atmosphere), the reader is advised to consult references (IMAGE, 2023; premise, 2023; REMIND, 2023).

Figure 1-A2 presents results for two environmental impact categories ("climate change" and "resource use, minerals and metals") for the production of gaseous hydrogen via high-temperature electrolysis coupled with a concentrated solar power (CSP) plant. This system corresponds to that used as case study in the deliverable D6.3 of the SH2E project, which was based on the model provided in Puig-Samper et al. (2022). The impacts are shown for the different background databases used to perform the calculations. These databases, generated with *premise*, include (i) the conventional ecoinvent cut-off 3.8 database, (ii) a prospective version of the former for the year 2030, assuming a Shared Socioeconomic Pathway (SSP) 2 and no climate policies implemented (SSP2 Base 2030), and (iii) an additional prospective version for 2030, assuming the same SSP scenario but acknowledging the fulfilment of the Nationally Determined Contributions (NDCs) for climate change mitigation from the Paris Agreement (SSP2 NDC 2030).

Based on the results for climate change in Figure 1-A2, the linkage of the foreground system to the aforementioned databases has a very relevant effect. The results range from 3.5 kg CO_2-eq/kg H_2 when using retrospective background data (i.e. conventional ecoinvent) to 1.3 kg CO_2-eq/kg H_2 (a 63% reduction) when considering a more optimistic 2030 context (i.e. SSP2 NDC 2030). This variation can be especially critical when performing an LCA study for decision-making purposes, as restricting the analysis to the use of the conventional database could lead to misinterpretation regarding the qualification of hydrogen as renewable, e.g., when considering a threshold of 3.4 kg CO_2-eq/kg H_2 (Campos-Carriedo et al., 2023). Additionally, Figure 1-A2 shows how shifting to a decarbonised economy could increase impacts on mineral raw materials depletion. Again, restricting the assessment to the use of a conventional background database could entail losing insights into the implications of transitioning from fuel-intensive to material-intensive energy systems (International Energy Agency, 2021).

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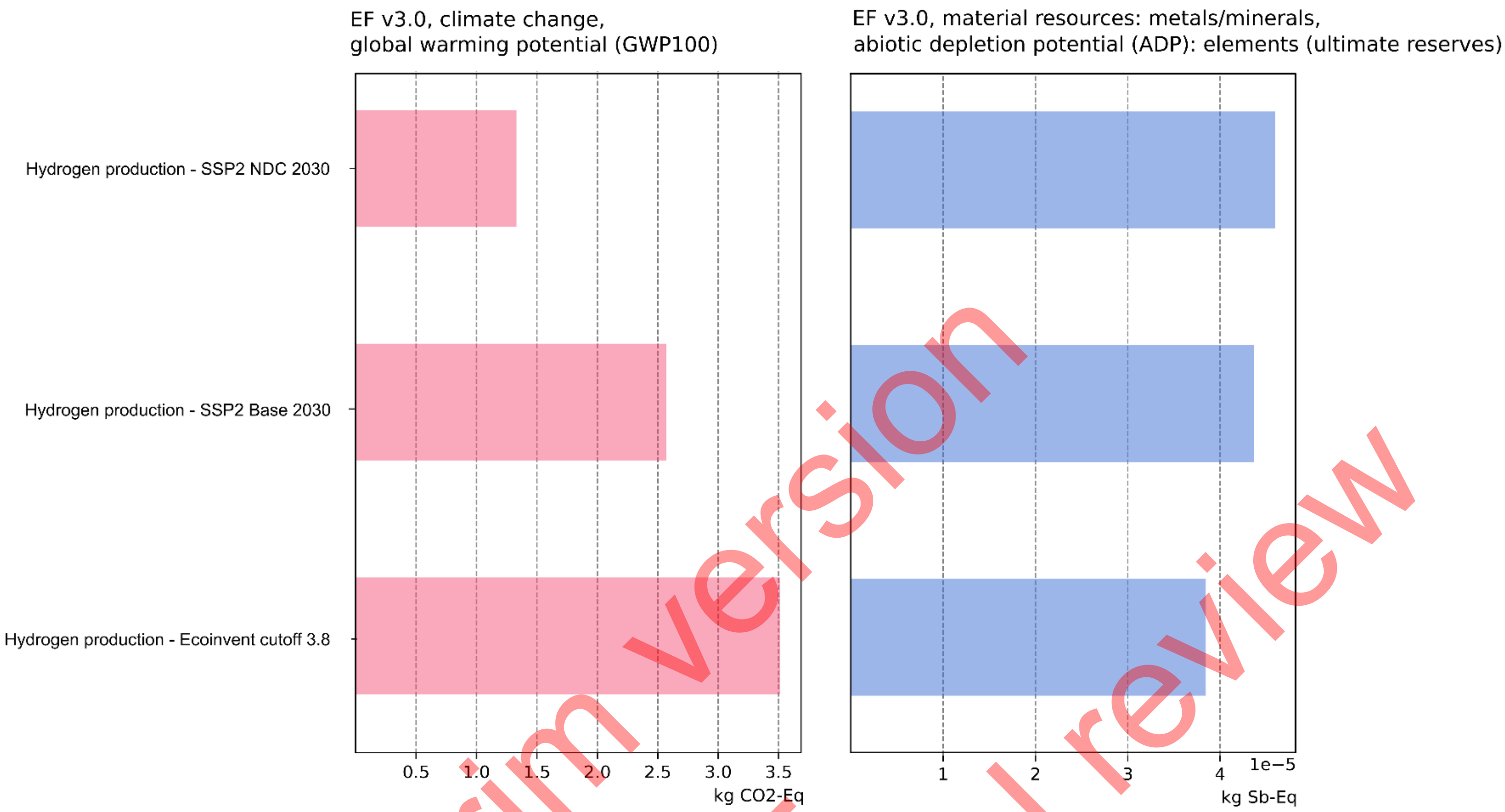

Figure 1-A2. Influence of the background database on the prospective environmental performance of hydrogen produced via high-temperature electrolysis.

REFERENCES

Campos-Carriedo F, Bargiacchi E, Dufour J, Iribarren D. How can the European Ecodesign Directive guide the deployment of hydrogen-related products for mobility? Sustain Energy Fuels 2023;7:1382-94. https://doi.org/10.1039/D2SE01486F.

IMAGE. IMAGE 3.2 Documentation. https://models.pbl.nl/image/index.php/Welcome_to_IMAGE_3.2_Documentation (accessed Aug. 30, 2023).

International Energy Agency. The Role of Critical Minerals in Clean Energy Transitions. OECD, May 2021. https://doi.org/10.1787/f262b91c-en.

premise. premise 1.5.0-alpha documentation. https://premise.readthedocs.io/en/latest/index.html (accessed Aug. 30, 2023).

Puig-Samper G, Bargiacchi E, Iribarren D, Dufour J. Assessing the prospective environmental performance of hydrogen from high-temperature electrolysis coupled with concentrated solar power. Renew Energy. 2022; 96:1258–1268. https://doi.org/10.1016/J.RENENE.2022.07.066.

REMIND. REMIND — Potsdam Institute for Climate Impact Research.” https://www.pik-potsdam.de/en/institute/departments/transformation-pathways/models/remind (accessed Aug. 30, 2023).

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ANNEX 3 - LIFE CYCLE ASSESSMENT OF HYDROGEN FOR SPECIALTY GLASS PRODUCTION: COMPARING HYDROGEN HEATING WITH CONVENTIONAL NATURAL GAS HEATING

1. GOAL OF THE LIFE CYCLE ASSESSMENT

The **goal** of this LCA study is to evaluate the environmental profile of specialty glass production with a hydrogen heating system in 2020, 2030 and 2050 in Germany. The focus is on the use of hydrogen for high-temperature heat production in industry, rather than on the actual glass production.

Two hydrogen supply options were analysed (i) centralised hydrogen production in large scale polymer electrolyte membrane (PEM) electrolysers and subsequent transport to the specialty glass production plant with liquid organic hydrogen carrier (LOCH), and (ii) onsite hydrogen production at the glass production plant with a smaller scale PEM electrolyser. For selecting the appropriate **benchmark technology** for this case study, a look at the current situation in Germany is helpful. According to Leisin (2020), mainly natural gas is used for fuelling glass production in Germany (>95%). A few plants still use heating oil as a fuel and few plants operate fully electric. Thus, selecting a natural gas heating system for glass production is advised. For all three options an oxyfuel burner needing additional oxygen was used.

Although the progressive implementation of new hydrogen pathways is expected to have a large scale-effect, this study places the focus on accounting for the potential environmental impacts of the specific specialty glass product, with decision-support limited to the specific product (i.e. micro-level decision support). A **prospective attributional** life cycle inventory (LCI) modelling approach was chosen. The present LCA study is not meant for decision making at meso or macro level, as it aims at defining the prospective environmental profile of specialty glass with hydrogen heating comparing it to that of conventional specialty glass production with natural gas heating. Moreover, this study should be understood as case-specific.

2. SCOPE OF THE LIFE CYCLE ASSESSMENT

2.1 Modelling approach

The current LCA study places the focus on defining the environmental profile of specialty glass produced with a hydrogen heating system. As the supply options for hydrogen will further develop over the next decades, the system was modelled for 2020, 2030 and 2050 to appropriately explore the potential of hydrogen for high-temperature heat production in industry. In this sense, the present LCA was approached from a **prospective point of view**. Since this study does not aim at guiding decision making at meso or macro level, consequentiality topics were not addressed herein.

2.1.1 Prospectivity

The system under evaluation was modelled based on the years 2020, 2030 and 2050, when it is expected that hydrogen supply chains will reach full technical maturity. Thus, the hydrogen supply of the system was modelled according to the expected technical performance indicators for the respective years (e.g. efficiency, cell degradation rate, and fuel for truck transport) based on experts' opinions. The modelling of glass trough operation with hydrogen and the benchmark with natural gas were based on process simulations.

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External electricity demand linked to the foreground system for the years 2030 and 2050 were modelled with a prospective electricity mix based on the results of an energy system model.

2.2 Functional unit

The only function of the system is to produce specialty gas. Hence, only one functional flow was involved. The **functional unit** (FU) of the study was defined as the production of 1870 kg of specialty glass corresponding to the production of one hour. Although hydrogen and oxygen are produced during the PEM electrolysis, no allocation was carried out between the two products. At the central hydrogen production facility, oxygen was considered as waste and no allocation was necessary; at the glass production plant, it is used for operating the oxyfuel burner.

The FU of the competing system for benchmarking (natural gas heating for specialty glass production) was also defined as 1870 kg of specialty glass at the same above-mentioned conditions.

2.3 System boundaries

The system boundaries of the study encompass all life-cycle phases of the system under evaluation from raw material extraction to glass production (Figure 1-A3). The production system involves two main sections: (i) **hydrogen supply**, and (ii) **operation of the glass** trough. However, all capital goods and material flows that stay the same for all analysed glass production options were not considered, e.g., silica and lime as feedstock for the glass as well as the glass trough as capital good.

For hydrogen supply, two different options were considered: (i) centralised hydrogen production with subsequent transport in LOHC, and (ii) onsite hydrogen production. For hydrogen transport with LOHC, the hydrogen is chemically bound to an LOHC, here benzyl toluene (BT) during a hydrogenation process. For the release of hydrogen (dehydrogenation), additional heat is necessary (Rüde et al., 2022). At the same time, the glass production releases waste heat. This waste heat is used for the dehydrogenation of hydrogen from BT. As this amount of heat is not fully sufficient for dehydrogenation, extra electric heating is necessary. Onsite hydrogen production with PEM electrolysis not only provides hydrogen for the oxyfuel combustion, but also oxygen. However, as the oxyfuel combustion is run under excess air conditions, still some oxygen needs to be produced by an air separation unit.

Processing and use of specialty glass for a specific industrial application is out of the presented scope. Decommissioning of the production units or other end-of life processes were neglected. No cut-off was applied.

Capital goods (without EoL) directly relevant to the entire foreground system under evaluation (e.g. PEM electrolyser and air separation unit) were included in this analysis. The lifetime of the system was assumed to be 20 years, except for the PEM stacks, which improve over the years from five to ten years. Capital goods belonging to the background processes (e.g. for electricity generation) were considered relying on the information provided by the selected background database (ecoinvent v.3.6).

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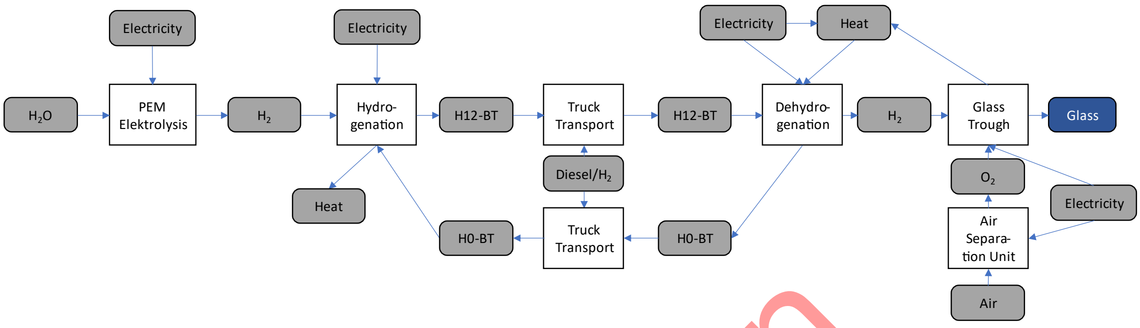

Figure 1-A3. System boundary of the LCA for specialty glass production with hydrogen supplied by Liquid Organic Hydrogen Carrier (LOHC) [BT: benzyl toluene, PEM: polymer electrolyte membrane] (Wulf and Zapp, 2023).

2.4 Multi-functionality

It was assumed that, for oxygen produced together with hydrogen during electrolysis, there is no possibility of external use. Furthermore, the heat produced during specialty glass production was considered as waste if not used internally. Thus, there is no multi-functionality to consider.

3. LIFE CYCLE INVENTORY

The LCI corresponding to the modelling of the foreground system was retrieved from a work previously developed within the context of the German Kopernikus project (Ausfelder and Tran, 2022).

3.1 Data sources and availability

Most of the LCI data of the specialty glass production (foreground data) were provided by Kopernikus project partners:

1. PEM electrolyser:
   - Technical University Munich.
2. LOHC technology:
   - Hydrogenious LOHC Technologies GmbH.
3. Specialty glass production:
   - Schott AG.
4. Energy system models:
   - Technical University Munich.
   - Ostbayerische Technische Hochschule Regensburg.

For the **background processes** (e.g. electricity and water supply), the ecoinvent 3.6 database (system model “Allocation, cut-off by classification”) was used. The complete LCI of the foreground and background system is provided in Wulf and Zapp (2023).

The German electricity mixes used in this study are summarised in Table 1-A3. The future scenarios are complying with the current climate goals of the German government and will reach climate neutrality by 2045.

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Table 1-A3. Composition of the German electricity mix in different years (Bauer et al., 2022).

Energy carrier	2020	2030	2050
Biomass	10%	8%	1%
Hard coal	7%	-	-
Natural gas	17%	7%	0%
Hydropower	4%	4%	2%
Lignite	16%	-	-
Photovoltaics	10%	12%	29%
Wind, offshore	5%	23%	20%
Wind, onshore	20%	24%	24%
Mineral oil	1%	-	-
Nuclear power	12%	-	-
Import	-	23%	24%

4. LIFE CYCLE IMPACT ASSESSMENT

The Life Cycle Impact Assessment (LCIA) method package selected for the study was the **Environmental Footprint version 3.1**, published by the Joint Research Centre (JRC). Table 2-A3 provides an overview of the midpoint environmental impact categories and indicators included in EF 3.1, their reference units, and the corresponding results of the specialty glass production related to 1870 kg of specialty glass produced (FU) over the years. Figure 2-A3 shows a graphic representation of the climate change results. In the current scenario, the results are dominated by the hydrogen production emissions. Therefore, the conventional heating of the glass tank with natural gas causes significantly lower amounts of greenhouse gas emissions than the hydrogen options. Within the hydrogen options, however, significant differences emerge. Onsite hydrogen production benefits not only from not needing transportation but also from oxygen production. Oxygen is produced as a by-product of electrolytic hydrogen production, meaning that little additional oxygen needs to be produced for combustion through air separation. At the same time, as greenhouse gas emissions from electricity decline, hydrogen heating becomes competitive with conventional natural gas heating from a climate perspective.

As discussed above, significant climate change benefits are possible from hydrogen heating for specialty glass production. However, as shown in Figure 3-A3, this is not true for all environmental impacts analysed. In particular, resource use, particulate matter and acidification increase sharply when hydrogen heating is used. This is significantly related to the electricity-based hydrogen production. In addition, electricity is also needed to condition the hydrogen for transport. Onsite hydrogen production is the best alternative regarding water use, in addition to climate change. For water use, low results can be achieved because almost the entire oxygen demand of the glass production is covered by the electrolysis and the water for cooling the air separation unit is saved. For the acidification and particulate emissions categories, natural gas use remains a better alternative.

No normalisation, grouping or weighting of impact categories was performed.

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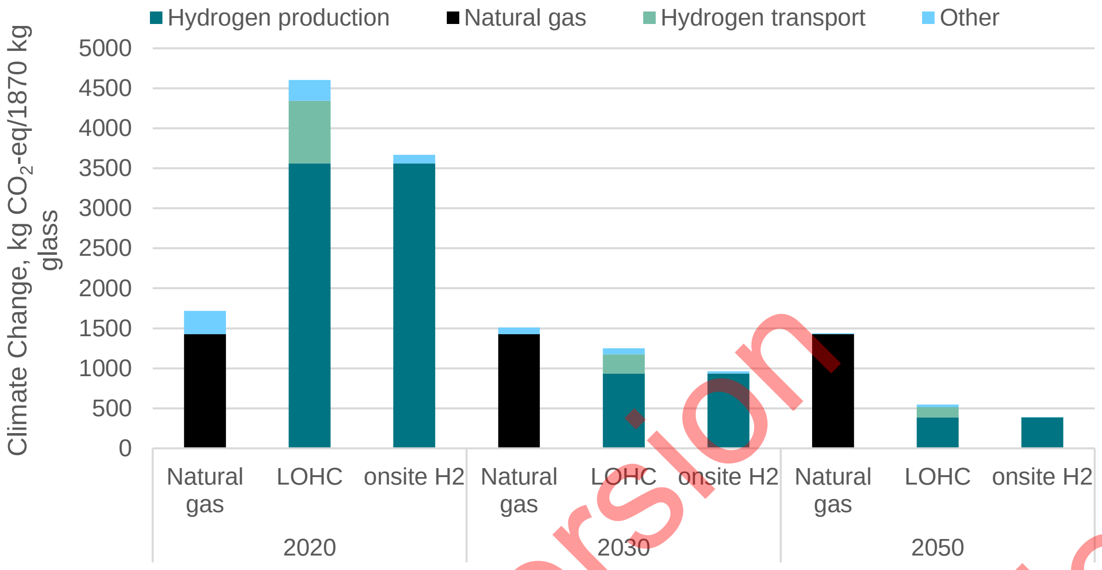

Figure 2-A3. Climate change impacts of 1870 kg of glass with different heating options for three points in time.

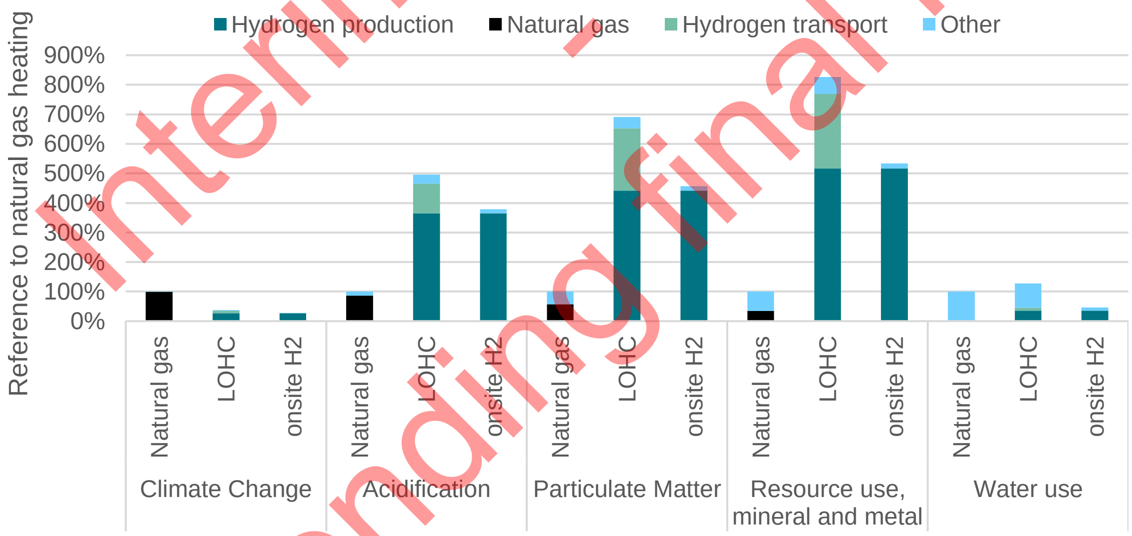

Figure 3-A3. Trade-offs of selected environmental impact categories for specialty glass production (heating with natural gas as a reference) in 2050.

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Table 2-A3. LCIA results to produce 1870 kg of glass with different heating options according to the EF3.1 method package.

Impact categories and indicators	Unit	2020	2020	2020	2030	2030	2030	2050	2050	2050
		Natural gas	LOHC	Onsite	Natural gas	LOHC	Onsite	Natural gas	LOHC	Onsite
Acidification	mol H^+ eq	1.72E+00	1.47E+01	1.17E+01	1.33E+00	8.01E+00	6.25E+00	1.11E+00	4.48E+00	3.42E+00
Climate change	kg CO_2 eq	1.72E+03	4.60E+03	3.67E+03	1.51E+03	1.25E+03	9.64E+02	1.46E+03	5.47E+02	4.02E+02
Climate change – Biogenic	kg CO_2 eq	7.68E+00	1.12E+02	9.25E+01	7.06E+00	9.76E+01	7.82E+01	1.85E+00	2.07E+01	1.65E+01
Climate change – Fossil	kg CO_2 eq	1.71E+03	4.49E+03	3.58E+03	1.50E+03	1.14E+03	8.78E+02	1.46E+03	5.21E+02	3.81E+02
Climate change – Land use and LU change	kg CO_2 eq	2.85E+02	4.33E+03	3.57E+03	7.63E-01	9.38E+00	7.46E+00	5.33E-01	5.64E+00	4.45E+00
Ecotoxicity, freshwater	CTUe	1.44E+03	1.39E+04	1.08E+04	8.49E+02	3.85E+03	3.08E+03	9.22E+02	4.60E+03	3.42E+00
Ecotoxicity, freshwater – inorganics	CTUe	1.42E+03	1.36E+04	1.07E+04	8.27E+02	3.69E+03	2.98E+03	8.98E+02	4.42E+03	4.02E+02
Ecotoxicity, freshwater – organics	CTUe	2.61E+01	3.14E+02	1.69E+02	2.20E+01	1.61E+02	1.08E+02	2.41E+01	1.78E+02	1.65E+01
Energy resources: non-renewable	MJ net calorific value	2.80E+04	6.98E+04	5.55E+04	2.50E+04	2.19E+04	1.68E+04	2.41E+04	7.87E+03	5.60E+03
Eutrophication, freshwater	kg P eq	4.16E-01	5.63E+00	4.63E+00	6.57E-02	2.96E-01	2.15E-01	1.11E+00	3.38E-01	3.65E+03
Eutrophication, marine	kg N eq	6.04E-01	3.38E+00	2.63E+00	4.59E-01	1.03E+00	7.38E-01	1.46E+03	7.24E-01	3.53E+03
Eutrophication, terrestrial	mol N eq	6.97E+00	4.35E+01	3.41E+01	6.05E+00	2.67E+01	2.06E+01	1.85E+00	1.05E+01	1.22E+02
Human toxicity, cancer	CTUh	1.94E-07	1.04E-06	7.88E-07	1.81E-07	8.47E-07	5.74E-07	1.46E+03	9.59E-07	2.48E-01
Human toxicity. cancer – inorganics	CTUh	8.34E-08	7.10E-07	5.39E-07	6.79E-08	4.90E-07	3.16E-07	5.33E-01	5.60E-07	5.01E-01
Human toxicity. cancer – organics	CTUh	1.10E-07	3.30E-07	2.49E-07	1.13E-07	3.57E-07	2.57E-07	9.22E+02	3.99E-07	7.66E+00
Human toxicity, non-cancer	CTUh	3.75E-06	3.68E-05	2.90E-05	2.74E-06	2.14E-05	1.50E-05	8.98E+02	2.65E-05	6.67E-07
Human toxicity. non-cancer – inorganics	CTUh	3.51E-06	3.57E-05	2.82E-05	2.51E-06	2.04E-05	1.43E-05	2.41E+01	2.55E-05	3.75E-07
Human toxicity. non-cancer – organics	CTUh	2.32E-07	1.06E-06	8.05E-07	2.30E-07	9.99E-07	7.13E-07	7.03E-02	9.54E-07	2.93E-07
Ionising radiation	kBq U-235 eq	8.42E+01	8.38E+02	6.81E+02	4.78E+01	2.63E+02	2.07E+02	4.42E-01	9.73E+01	1.92E-05
Land use	-	2.65E+03	3.56E+04	2.72E+04	2.96E+03	3.75E+04	2.86E+04	4.98E+00	5.34E+04	1.85E-05
Ozone depletion	kg CFC11 eq	2.23E-04	3.61E-04	2.73E-04	2.15E-04	1.86E-04	1.44E-04	1.93E-07	5.73E-05	6.78E-07
Particulate matter	disease inc.	9.35E-06	9.06E-05	6.35E-05	8.57E-06	7.09E-05	4.92E-05	7.55E-08	5.19E-05	7.45E+01
Photochemical ozone formation	kg NMVOC eq	1.81E+00	6.89E+00	5.11E+00	1.61E+00	3.18E+00	2.29E+00	1.18E-07	2.38E+00	4.13E+04
Material resources: metals/minerals	kg Sb eq	1.29E-03	9.27E-03	5.62E-03	1.39E-03	1.08E-02	6.33E-03	1.68E-03	1.39E-02	9.00E-03
Water use	m^3 depriv.	1.65E+03	2.13E+03	8.14E+02	1.65E+03	2.07E+03	7.40E+02	1.66E+03	2.09E+03	7.60E+02

Clean Hydrogen Partnership

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5. INTERPRETATION AND FINAL REMARKS

It was shown that, for the industrial specialty glass production in Germany, a heating system with electrolytical hydrogen – even with hydrogen that is not green – is more climate friendly in 2030 and the years to follow than conventional natural gas heating. Taking the long investment cycles in the industry into consideration, already today such systems must be further explored. Regarding the different options for hydrogen supply from a climate perspective, onsite electrolysis is the best option. Not only the hydrogen from the PEM electrolyser can be used, but also the simultaneously produced oxygen for the oxyfuel combustion.

However, when looking beyond climate change, there are several trade-offs regarding other environmental impacts. Resource use will be at least five times higher. Further analyses are necessary to evaluate the sources of these high demands as well as their severity. In addition, measures need to be discussed to mitigate the impacts of acidification and particulate matter. It is advised to include further prospectivity aspects of the background system, for example for steel or cement production.

Before installing a hydrogen heating system, it should be checked if a direct electrification is another technically viable option or at least a hybrid system combining electric and hydrogen heating, because electric melting is more efficient than hydrogen-based systems (Wulf and Zapp, 2023).

REFERENCES

Ausfelder F, Tran DD. 4. Roadmap des Kopernikus-Projektes P2X - Phase II - Optionen für ein nachhaltiges Energiesystem mit Power-to-X Technologien: Transformation – Anwendungen – Potenziale. Frankfurt am Main: DECHEMA 2022.

Bauer F, Gawlick J, Sterner M, Hamacher T. Einbettung der Analysen in den Gesamtkontext der Energiewende und Klimaschutzziele - Übergreifende Energiesystemmodellierung. In: Ausfelder F, Tran DD, editors. 4 Roadmap des Kopernikus-Projektes P2X Phase II - Optionen für ein nachhaltiges Energiesystem mit Power-to-X Technologien. Frankfurt am Main: DECHEMA; 2022.

Leisin M. Energiewende in der Industrie: Potenziale und Wechselwirkungen mit dem Energiesektor - Branchensteckbrief der Glasindustrie. Berlin: German Federal Ministry for Economic Affairs and Energy; 2020.

Rüde T, Dürr S, Preuster P, Wolf M, Wasserscheid P. Benzyltoluene/perhydro benzyltoluene – pushing the performance limits of pure hydrocarbon liquid organic hydrogen carrier (LOHC) systems. Sustainable Energy & Fuels 2022;6:1541-53.

Wulf C, Zapp P. Environmental Impacts of Using Hydrogen for Defossilizing Industrial Specialty Glass Production. In: Schossig P, Droege P, Riemer A, Speer M, editors. Proceedings of the International Renewable Energy Storage Conference (IRES 2022). Düsseldorf: Atlantis Press; 2023. p. 538-50.

ANNEX 4 - SUPPLY CHAIN MODELLING WITH DIFFERENT SCOPES IN SLCA

This annex illustrates potential issues regarding supply chain definition in life-cycle studies. In particular, an SLCA case study of a 48 kW Proton Exchange Membrane Fuel Cell (PEMFC) stack is used for illustrative purposes. Bargiacchi et al. (2022) addressed the SLCA of one 48 kW PEMFC stack based on a supply chain defined according to a protocol for product social life cycle assessment (Martín-Gamboa et al., 2020), assuming Spain as the manufacturing country. The resultant product-specific supply chain involved three tiers: a first one referring to the stack manufacturing plant, another involving the plants related to the production of the stack components and the energy flows required by the aforementioned tier, and a final one containing the plants where the materials and energy flows required by the second tier are produced. In the original study, in order to preserve the product specificity of the supply chain, it was not extended by considering upstream interactions at the sector level. This annex explores the influence of such a choice.

In Figure 1-A4, the identification of contributors to six social indicators for the manufacturing of one 48 kW PEMFC stack is shown. The coloured boxes represent the top-five contributors, from red (indicating the most impactful process) to light yellow (representing the fifth most impactful process). The analysis distinguishes between contributions stemming from the activities within the product system as assessed in Bargiacchi et al. (2022) (i.e. **product-specific supply chain**, labelled "Product" in the figure) and those originating from the upstream generic sectoral interactions that could be additionally linked to its last product-specific tier (i.e. **sector-extended supply chain**, labelled "Full system"). A product-specific system in SLCA (which could often be understood as an extended foreground system in conventional LCA) is understood herein as that in which its supply chain is built upon the combined use of LCA unit process datasets (to identify the exchanges that correspond to each product-specific activity) and primary or secondary trade data (to identify the location/countries in which these activities take place). On the other hand, sector-extended systems complete the definition of the supply chain by relying on upstream sectoral interactions provided by SLCA databases such as PSILCA in an attempt to reach the depth typically achieved in LCA, at the expense of losing specificity at the product level.

Overall, incorporating the upstream sectoral interactions in the SLCA model was found to have a substantial effect on the magnitude of the social impacts observed across the six indicators. However, even with this sector-extended perspective, the unit process with the highest impact remains situated within the confines of the product-specific supply chain. This is, in five out of the six indicators, platinum production in South Africa. Moreover, other processes within the product-specific supply chain also play an important role as top-five contributors to the fair salary, forced labour, and health expenditure indicators.

A detailed tree-grouping analysis using the functionalities of openLCA reveals that the key contributors outside the restricted product system predominantly converge into the most influential activity (highlighted in red). This implies that focusing the assessment on the product-specific supply chain does not lead to a loss of insights into which stages of the supply chain require special attention, while ensuring a product-specificity level comparable to an LCA study (which is envisaged as a key aspect when conducting an SLCA study of FCH technologies, as they tend to rely on evolving supply chains that might not be suitably modelled by generic interactions at the sector level).

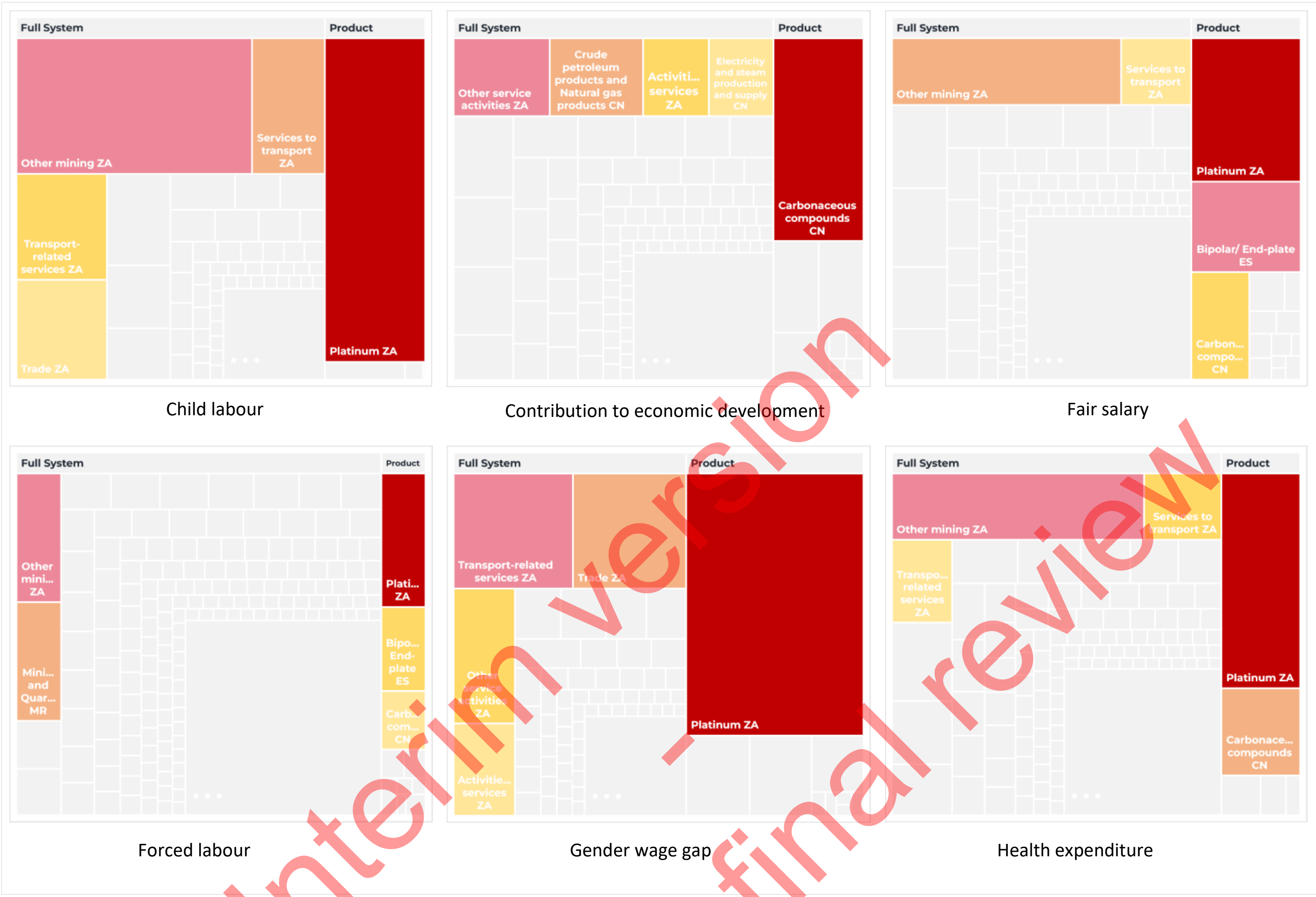

Figure 1-A4. Contributors to social impacts across product-specific (labelled as "Product") and sector-extended (labelled as "Full system") supply chains for the manufacturing of one 48 kW PEMFC stack.

REFERENCES

Bargiacchi E, Campos-Carriedo F, Iribarren D, Dufour J. Social life cycle assessment of a proton exchange membrane fuel cell stack. E3S Web of Conferences 334, 09001. 2022. https://doi.org/10.1051/e3sconf/202233409001.

Martín-Gamboa M, Dias AC, Arroja L, Iribarren D. A protocol for the definition of supply chains in product social life cycle assessment: application to bioelectricity. Sustainable Energy & Fuels 2020;4:5533-42. https://doi.org/10.1039/D0SE00919A.

ANNEX 5 - BIOGENIC CARBON EMISSIONS AND STORAGE

Susmozas et al. (2016) conducted an LCA study to evaluate the life-cycle performance of hydrogen produced via indirect biomass gasification with CO_2 capture. The poplar gasification system with CO_2 capture ("PG&C system") produces hydrogen and carbon dioxide. In this study, 100% of the environmental burdens were allocated to the main product of the system: hydrogen. Regarding the carbon cycle, a negative carbon footprint result was obtained, which means that the bioenergy system provided with CO_2 capture under study would succeed in attaining net carbon fixation due to the CO_2 uptake during the cultivation phase. In this study, a carbon neutral cycle modelling was carried out applying -1 to uptake and 1 to CO_2 emission. A concern regarding this article within the SH2E guidelines refers to the assignment of carbon credits. In this case, the original study followed a cradle-to-gate scope that did not include the storage of CO_2. In order to be SH2E compliant, the analysis should be extended to include CO_2 storage, with a carbon storage time higher than 100 years.

REFERENCES

Susmozas A, Iribarren D, Zapp P, Linßen J, Dufour J. Life-cycle performance of hydrogen production via indirect biomass gasification with CO_2 capture. Int J Hydrogen Energy 2016; 41(42):19484-19491. https://doi.org/10.1016/j.ijhydene.2016.02.053.

ANNEX 6 - PSILCA WORKER HOURS DATABASE VS. RAW VALUES (DIRECT QUANTIFICATION) DATABASE

Regarding the Product Social Impact Life Cycle Assessment database (PSILCA) (Loubert et al., 2023), two approaches of the database exist (cf. the FCH-SLCA guidelines developed in the SH2E project, D4.2): one relying on the **activity variable worker hours** (WH – worker hours approach) and one **without an activity variable**, but with a direct quantification approach instead (RV – raw values approach). The application of the two approaches is described and compared herein for an example of a fuel cell electric vehicle (FCEV).

The social data – raw indicator values – used for the assessment are the same for both databases. If the indicators gender wage gap and trade union density are to be assessed, data for each unit process inside the product system are to be gathered. For example, the gender wage gap of the FCEV production can be primary data, if available, or generic, taken from the German sector "Passenger cars and parts", from the PSILCA database. PSILCA retrieves these data from ILOSTAT (ILO, 2019).

In the WH approach, the raw indicator values are translated into **risk levels**, with the help of reference scales, defined by GreenDelta, the developers of PSILCA, which can be adjusted by the practitioner (Loubert et al., 2023). For a gender wage gap of 20.87% (German values), the risk level is 'high risk'; and a trade union density of 17 % (German value) poses a 'very high risk'. The risk-assessed indicators do not have quantitative values anymore, but a qualitative attribute in the form of risk levels. The quantitative amount of the indicators are the worker hours needed for one unit process, e.g., 12 h for the final FCEV assembly. Thus, the indicators are written as, e.g., "Gender wage gap, high risk, 12 h" and "Trade union density, very high risk, 12 h". In the RV approach, the raw indicator values are used directly in the calculation, without risk levels and worker hours.

All risk-assessed indicators, the worker hours assigned, and economic values form the inventory of the WH approach, i.e., the whole set of data needed for the calculation, whereas in the RV approach, the inventory consists of the indicator raw values and the economic values only. The first part of the calculation, the inventory results, is the same for both databases. Follow-up calculations differ.

In the WH approach, these follow-up calculations consist of an impact assessment. The inventory results are multiplied by characterisation factors, which have the unit medium risk hours per hour and are specific to an impact category (cf. Section 4.1 of the present FCH-LCSA guidelines). The characterisation factors are defined for each risk level (Loubert et al., 2023); in the case discussed above, 10 for a high risk and 100 for a very high risk, which are then multiplied by the social indicator value and a conversion factor for the unit, e.g., 0.5 d * 10 gender wage gap med risk hours/h * 24 h/d = 120 gender wage gap med risk hours.

In the RV approach, inventory results on an indicator level undergo a normalisation procedure, which is the weighted average of the indicator raw value (cf. SH2E deliverable D4.2). The indicator raw values of the inventory as well as the normalised results can have different units, according to the indicator measured, e.g., % for gender wage gap and trade union density or USD for minimum wage. Compared to the WH approach, this can be easier to understand. The indicator raw values (e.g. gender wage gap 20.87% in Germany and trade union density 17% in Germany) are used directly in the calculation, without risk levels or worker hours.

Due to the different calculation procedures of the two approaches, also the modelling requirements are different. Neither of these requirements are beneficial or adverse, but important to keep in mind while modelling a product system in the respective database.

In the WH approach, a unit process can be modelled without adding any social indicator flow, if it is a bridge process, i.e., a unit process not provoking any social impacts. This is not possible in the RV approach. Social indicator flows have to be added to every unit process and, in addition, they have to be the same across the whole product system. Another requirement is the modelling of a unit process with an output flow equalling 1 USD in the RV approach, whereas in the WH approach, the reference flow can have any amount and unit (Loubert et al., 2023). The third one is a consequence of the first two requirements in the RV approach: every unit process contributes to the results, i.e., the number of unit processes has an influence on the results.

The results of the WH approach can be interpreted on an indicator as well as on an impact category level. They are specific for every indicator and impact category, i.e., FS medium risk hours for the impact category fair salary cannot by compared with CL medium risk hours for the impact category child labour (Loubert et al., 2023). The results of the WH DB in the units of indicator specific medium risk hours can only be assessed for comparative systems, e.g., comparing FS medium risk hours of a battery electric vehicle with FS medium risk hours of an FCEV (presupposing that they have the same functional unit, system boundaries approach, etc.).

In the RV approach, the results can also be assessed in comparison to a product system of the same functional unit, etc. As the results are expressed in their underlying unit, also a straightforward interpretation becomes possible. To ensure an objective evaluation, benchmarks are a useful tool to further assess the results. For example, a result for the indicator gender wage gap of 20.2 % for an FCEV can be compared to the gender wage gaps of different countries, e.g., by data from the World Economic Forum (2023) or even on a sectoral level by ILOSTAT (ILO, 2023).

REFERENCES

ILO - International Labour Organization. ILOSTAT database of labour statistics 2019. https://ilostat.ilo.org/data/. Geneva, Switzerland.

ILO - International Labour Organization. Data - Indicator catalogue.https://ilostat.ilo.org/data/#. Geneva, Switzerland.

Loubert M, Maister K, Di Noi C, Radwan L, Ciroth A, Srocka M. PSILCA v. 3.1. A Product Social Impact Life Cycle Assessment database. Documentation. Berlin, Germany. 2023.

World Economic Forum. Global Gender Gap Report 2023. Cologny/Geneva, Switzerland. 2023.

ANNEX 7 - APPLICATION OF THE SH2E RESOURCE INDICATOR TO MANUFACTURING OF DIFFERENT WATER ELECTROLYSIS CELLS

1. BACKGROUND

Given the relevance of addressing **material criticality** in the life cycle of FCH systems, a newly defined indicator was developed in the SH2E project. Following the logic of LCA, characterisation factors (*CF*) are defined to link the amount of materials being used with their criticality. Based on the **criticality assessment of the European Commission** (EC) an indicator considering the Supply Risk (*SR*), the material consumption (*C*) in the EU, the import reliance (*IR*), and the recycling input rate (EoL_{RIR}) was proposed (Bargiacchi et al., 2022; Zapp and Schreiber, 2021). High consumption poses a high risk if the EU relies heavily on imports of this material, and it is not recycled within the EU.

2. METHOD

The *CF* is derived by Equation (1):

$$CF = \frac{SR}{C * (1 - IR * (1 - EoL_{RIR}))} \tag{1}$$

Values for *SR, IR*, EoL_{RIR}, and *C* are provided by the EC critical raw material (CRM) list and the associated factsheets (European Commission, 2023; Screen Project 2023), which are updated and released every three years. If those values are provided for extracted materials and processed materials, the higher value should be chosen.

According to Equation (2), the final criticality indicator is the product of the mass *M* of a material *m* of the foreground system and the CF, considering all materials (critical and non-critical) addressed by the EC:

$$Criticality_m = M_m * CF_m \tag{2}$$

Following the recommendations in the FCH-LCA guidelines regarding the use of Environmental Footprint (currently EF3.1) as the preferred impact assessment method package (Bargiacchi et al., 2022), the proposed criticality indicator should be aligned with the EF3.1 indicator “Resource use, minerals and metals”.

3. CASE STUDY

The manufacturing of 1 m^2 of cell area (functional unit, FU) for alkaline water electrolysis (AEL), proton exchange membrane electrolysis (PEM-EL) and solid oxide electrolysis (SOEC) was used as a case study to test the proposed criticality indicator. The parameters *SR, C, IR*, and EoL_{RIR} come from the EC list. The Life Cycle Inventory (LCI) data were taken from Zhao et al. (2020). Materials such as lanthanum strontium cobalt ferrite (LSCF), gadolinium-doped ceria (GDC) and yttria-stabilized zirconia (YSZ) were divided into individual elements. Table 1-A7 presents the numbers used for the assessment.

Table 1-A7. Parameters used for the assessment.

Resource	EF3.1 Resource use, kg Sb eq.	SR	C, t	IR	EoL$_{RIR}$
Chromium	4.43E-04	0.7	1.2E+06	0.42	0.21
Iron	5.24E-08	0.5	1.3E+08	0.05	0.31
Molybdenum	1.80E-02	0.8	2.9E+04	1	0.3
Nickel	6.53E-05	0.5	3.0E+05	0.75	0.16
Zirconium	5.44E-06	0.8	2.3E+05	1	0.12
Titanium	2.79E-08	1.6	1.0E+06	1	0.01
Platinum	2.22E+01	2.1	1.5E+02	1	0.12
Iridium	n.a.	3.9	9.2E-01	1	0.12
Aluminium	1.09E-09	1.2	1.5E+07	0.89	0.32
Barite	0	1.3	5.1E+05	0.74	0
Borate	0	3.6	4.2E+04	1	0.01
Cobalt	1.57E-05	2.8	1.8E+04	0.81	0.22
Manganese	2.54E-06	1.2	4.8E+05	0.96	0.09
Zinc	5.38E-04	0.2	1.9E+06	0.56	0.34
Lanthanum	n.a.	3.5	6.5E+02	0.8	0.01
Strontium	7.07E-07	2.6	4.9E+04	0	0
Cerium	n.a.	4.0	2.7E+03	0.8	0.01
Gadolinium	n.a.	3.3	1.1E+01	0.8	0.01
Yttrium	5.69E-07	3.5	5.1E+02	0.8	0.01
Silica sand	0	0.3	3.2E+07	0	0.01
Vanadium	7.70E-09	2.3	1.3E+04	0	0.06

4. RESULTS

Figure 1-A7 shows the results of the case study and allows a hotspot analysis within the three cell types. For AEL, only five materials are used, with nickel having the highest amount with more than 7 kg, followed by iron (1.6 kg), chromium (0.4 kg), molybdenum (0.06 kg), and zirconium (0.9 g). None of these materials exceeds the criticality thresholds of the EC CRM list. Only nickel is listed as a strategic material in the EC CRM 2023 list. The new SH2E indicator emphasises the criticality of nickel, although molybdenum has higher SR and IR. However, the higher EoL$_{RIR}$ lowers the latter two factors. As molybdenum has by far the highest CF in the resource depletion method, it is the strongest contributor to this impact category.

The manufacturing of PEM-EL cells requires, in addition to the materials used for AEL (with the exception of zirconium), titanium, platinum, and iridium. Titanium (9.7 kg) and iron (0.8 kg) together account for 96% of the total material. Although four materials are listed as critical (titanium, platinum, iridium) or strategic (nickel) according to the EC 2023 list, the very small amount (13 g) of iridium dominates when the SH2E criticality indicator is applied because the very low European consumption (*C*) of iridium compared to the other materials (Table 1-A7). Since *C* is in the denominator of the formula of the SH2E indicator (Equation (1)), the criticality indicator becomes high when *C* is small. Regarding EF 3.1 Resource use, platinum has the by far largest CF with 1000 kg Sb eq. followed by iridium with 140 kg Sb eq., which is reflected in Figure 1-A7.

With 18 different materials, significantly more materials are required for the manufacturing of SOEC cell than for AEL and PEM-EL. However, the SH2E indicator assigns the greatest importance only to the rare earths (such as lanthanum and yttrium), but especially gadolinium (Figure 1-A7). Once again, the very low EU consumption of gadolinium is the main driver for the SH2E indicator. Furthermore, all rare earths must be imported 100% and hardly any recycling takes place. Although chromium and zinc have similar CFs in EF 3.1 Resource use among the materials used for SOEC (Table 1), chromium contributes > 99% of the total result due to its significantly larger amount (chromium 3.4 kg; zinc 0.1 kg).

In summary, this case study shows that nickel and molybdenum for AEL, iridium for PEM-EL, and gadolinium for SOEC are critical hotspots for cell manufacturing in the EU. Since consumption (*C*) is in the denominator of Equation (1), the SH2E criticality indicator becomes high when *C* is small. The other parameters (IR, EoL_{RIR}) have a smaller effect on the overall result.

The results of resource depletion (EF3.1 indicator) differ from those for criticality, especially for PEM-EL and SOEC. This is not surprising, since both methods are based on different perspectives. Therefore, they should not be compared with each other, but should highlight two different aspects of resource use, the scarcity and the criticality aspect.

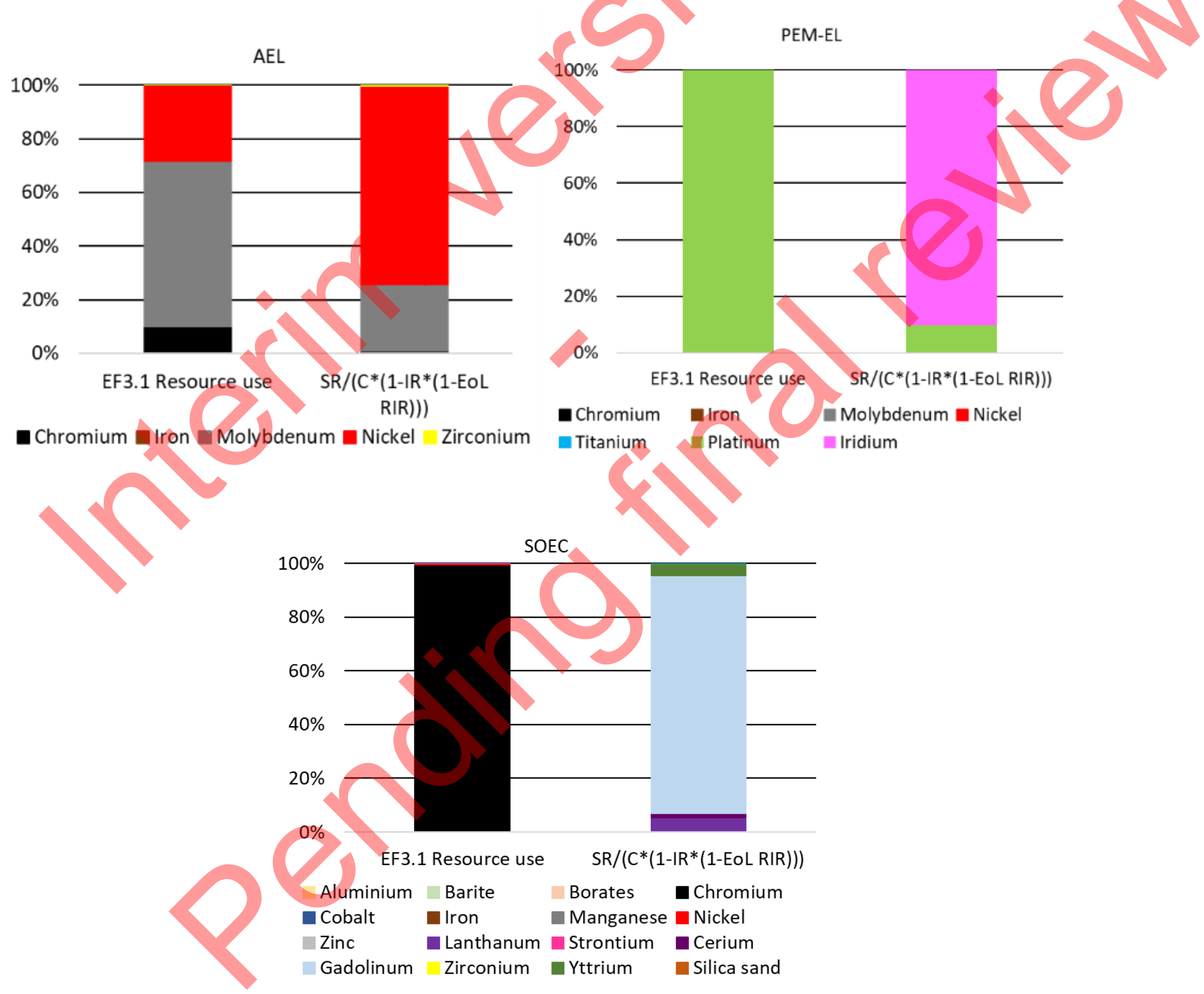

Figure 1-A7. Results of the new criticality indicator from SH2E and the resource depletion indicator considered in EF3.1 for the construction of 1 m² of cell area for three different electrolyser types.

It should be noted that, when using the impact category EF3.1 Resource use, some important materials for hydrogen technologies (such as iridium, rare earths) do not have characterisation factors in the underlying methodology (Abiotic Depletion Potential, from Institute of Environmental Sciences –CML– in 2017) (European Platform on LCA, 2022). For this reason, a comparison of the three cell types based on absolute values of the resource depletion indicator is not recommended for this case study.

Figure 2-A7 shows the comparison of the three cell types based on the absolute criticality values, which, in contrast to Figure (FU: 1 m^2 cell), were converted to 1 t of hydrogen production as reference unit. This allows a comparison between the three cell types including their different hydrogen production performance over their lifetimes. Hydrogen production of 19, 40, and 16 t was assumed over the lifetime of AEL, PEM-EL and SOEC, respectively (Zhao et al., 2020). As a result, it can be stated that the AEL performs better in terms of criticality (1.22E-05 points), of which about 85% is caused by nickel and 14% by molybdenum. The criticality of PEM-EL is significantly higher with approx. 1.3E-2 points for PEM-EL, followed by 2.5E-2 points for SOEC, which is almost double that of the PEM-EL. However, the criticality is mainly caused by different materials as already shown in Figure -A7 (iridium for PEM-EL, gadolinium for SOEC).

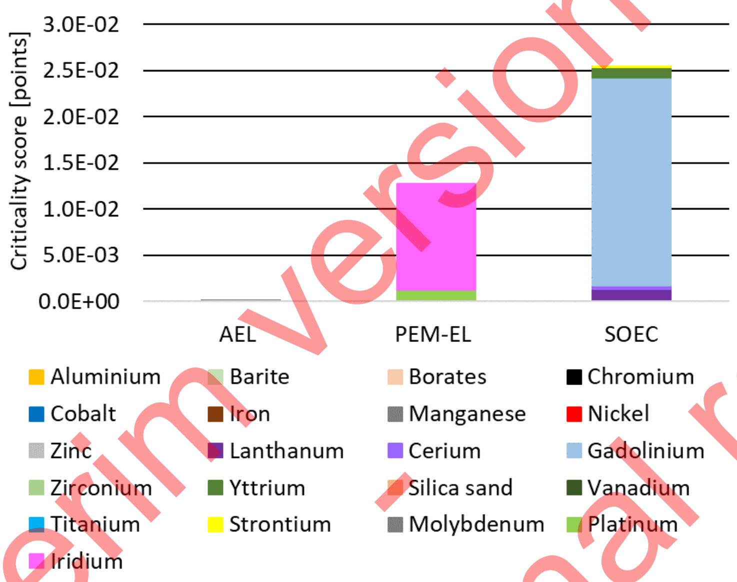

Figure 2-A7. Results of the new criticality indicator from SH2E to produce 1 t hydrogen using three different electrolyser types.

REFERENCES

Bargiacchi E, Puig-Samper G, Campos-Carriedo F, Iribarren D, Dufour J, Ciroth A, et al. D2.2 Definition of FCH-LCA guidelines WP2 Reformulation of current guidelines for Life Cycle Assessment. 2022.

European Commission, Directorate General for Internal Market, Industry, Entrepreneurship and SMEs, Grohol M, Veeh C. Study on the critical raw materials for the EU 2023 : final report: Publications Office of the European Union; 2023.

European Platform on LCA. EF reference package 3.1 (transition phase).https://eplca.jrc.ec.europa.eu/LCDN/developerEF.xhtml. Brussels: European Commission; last access: 27.07.2023. 2022.

Screen Project. Factsheets – CRMs 2023. Paris: Commissariat à l'énergie atomique et aux énergies (CEA); last access: 28.07.2023. 2023.

Zapp P, Schreiber A. D3.1 Material criticality indicator. Brussels: Clean Hydrogen Partnership; 2021.

Zhao G, Kraglund MR, Frandsen HL, Wulff AC, Jensen SH, Chen M, et al. Life cycle assessment of H2O electrolysis technologies. International Journal of Hydrogen Energy 2020;45:23765-81.

ANNEX 8 - CHALLENGES OF USING FUTURE ASSUMPTIONS AND DIFFERENT TRL TECHNOLOGIES IN LIFE CYCLE COSTING OF FCH TECHNOLOGIES

When conducting LCC of FCH technologies, practitioners often must use future assumptions or different TRL technologies compared with the current technology level. This is because most FHC products are currently under development and not yet on the market or the products on the market are expected to be improved in a short term. Therefore, the range of assumptions to be used will be large. This means data with a high degree of uncertainty or that only one data point is available when the technology is innovative.

Examples are:

- TRL of the product under development is low or there is no product on the market; therefore, practitioners must use CAPEX and OPEX speculated using analogous to similar products or facilities.
- Although products have been commercialised, their market is still small and not sufficient for providing precise data.
- Cost data in the literature are sometimes unclear in specifying the boundary.

With these data, both development of LCI and conversion to the economic value from LCI include uncertainty. When developing LCI with future assumptions, different conversion efficiencies and innovative processes influence LCI. When converting from LCI to an economic value (e.g. hydrogen cost), future unit costs of electricity, fuel and other consumables are proportional to each cost element in total hydrogen cost.

In all the above-mentioned cases, practitioners can understand the range of results by conducting sensitivity analysis with these assumptions in question so that they can screen which assumptions to be set carefully among uncertain ones. As shown in the figure, assumptions with high uncertainty and significant impact on the results should be set carefully, monitored and managed depending on the LCC objectives. Other data such as assumptions with high uncertainty and low impact on the result can be regarded as fixed assumptions.

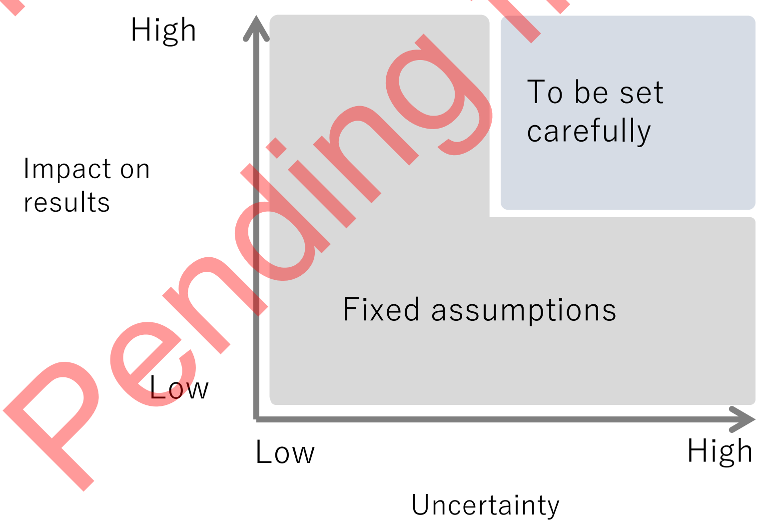

Figure 1-A8. Screening of assumptions to be set carefully by conducting sensitivity analysis.