Supplementary Information N°1 for

Harmonizing the assessment of (Green) Hydrogen Supply Chain: a modular and parametrized Life Cycle Assessment Framework.

Gabriel Magnaval [1,2,*], Maël Mouhoub [2], Anne-Marie Boulay[1], Manuele Margni[2]

[1] CIRAIG, Department of Chemical Engineering, Polytechnique Montreal, 2500 Chem. De Polytechnique, Montreal, Canada

[2] HES-SO Valais-Wallis, Rue de l'Industrie 21, Sion, Switzerland

[*] corresponding author details: gabriel.magnaval@polymtl.ca

Aim of this document

This document is a supplementary material dedicated to the critical analysis of the literature performed in the paper (section 2). It provides more details for each research gap identified, by explaining the problem and its consequence, and by indicating the literature sources illustrating the problem.

In the following section, a structured analysis of ten FC&EL LCA reviews [1–10], complemented by two additional methodological contributions[11,12] and thirty-three practical use cases [13–47] has been conducted (see **Supplementary Information SI1b** which compiles in a table the main elements of analysis for the 34 use cases). This analysis follows a three-step structure: (1) identification of the sources of methodological divergence that currently hinder the development of a consistent LCA framework; (2) examination of practitioners requirements from the LCA framework depending on their intended goals; (3) Comparison of these needs with the observed methodological gaps, and identification of potential solutions that will be explored in this paper to address the challenges and advancing the harmonization of LCA for FC&EL systems. The methodology and the results of this critical review are represented in Figure 1.

1. Sources of LCA methodological inconsistencies

This section outlined the sources of lack of harmonization identified in the critical review of existing LCAs on FC & EL technologies. These issues were grouped into two categories, following the ISO framework for LCA: research gaps related to the definition of the scope and to the modeling of the life cycle inventory.

1.1 Divergence in the scope of FC&EL LCA

According to ISO standards, defining the scope of an LCA involves establishing the functional unit— which quantifies the primary function of the system and serves as the basis for comparison—and identifying all processes necessary to fulfill this function. The scope must therefore align with both the technologies under study and their prospective functions. A key finding from the review is the lack of harmonization in scope definition across LCA studies, stemming from three main issues.

A diversity of functional units for the FC&EL LCA studies has been identified in the literature [4,6,7,10]. These functional units can be categorized into two groups: (a) those representing an intermediate product within the hydrogen supply chain, and (b) those capturing the final service delivered by the assessed technology. The first group includes units linked to system components—such as "kW of installed capacity" [17,35,41] or "m² of stack area" [20] - as well as units representing hydrogen production without specifying its application or the requirements to fulfill a downstream function. Hydrogen production is typically expressed with either mass-based ("1 kg of H_2 produced" [2,5,6,14,18,43]) or energy-based ("1 MJ or 1 kWh of H_2 produced" [13,16,44]) functional units. In contrast, the second group includes functional units that reflect the end-use of hydrogen, aligning more closely with its role in delivering a final service. For chemical applications, the functional unit has been set as "1 kg of hydrogen supplied at a specified pressure, temperature, and purity" [11,15,19,24,34,45–47] , highlighting that hydrogen produced, prepared and distributed to the consumer. Other examples include "1 vehicle-kilometer driven" or "1 ton-kilometer driven" for transportation applications [4,8,26,28,29], "1 MJ or 1 kWh of energy supplied" [7,12,25,27,32,36], or "1 kWh of electricity stored" [31,33] for energy carrier applications.
As studies become inherently difficult to compare when functional units differ, efforts toward harmonization are essential. While functional units must be tailored to the specific function of each hydrogen application, consistency within a given application—regardless of the technology assessed or the intended LCA goal—can be targeted. However, the coexistence of the two categories of functional units identified above (intermediate product-based vs. service-based) reveals that such harmonization is lacking, as studies assessing the same application may select a functional unit from either category.

Two main issues emerge regarding system boundaries. First, since system boundaries should reflect the functional unit and the context of the study, the diversity of functional units naturally leads to variability in which processes are included. Hydrogen supply chain processes such as compression, purification, storage, and distribution should be included when end-use functional units are defined but fall outside the system boundaries when intermediate product-based functional units are used [4,14,16,18,43,44]. Second, beyond these expected variations, the review highlights inconsistencies between the functional units defined and the system boundaries actually applied. In several cases, the supply chain processes (storage, distribution) are excluded without justification, even when they are necessary to fulfill the stated end-use function [4,6–9,36,39]. In addition, core components of the FC & EL systems are frequently omitted. This includes the balance-of-plant (BoP) (i.e. auxiliary equipment) essential for system operation [4,14,35,37,41], end-of-life treatment of the stack [4,14,24,37,42,43], or in rare cases, the stack itself [34]. Finally, at the stack level, core layers are sometimes excluded from the boundaries, such as the end-plates [13,37,39] or the current collectors [13,20,35,37,42]. These omissions compromise the representativeness and completeness of the assessments.

1.2 Divergence in the Life Cycle Inventory

According to ISO, the life cycle inventory (LCI) aims to quantify the flows which links the elementary processes in the system boundaries. This step requires describing how the elementary processes are linked, collecting data on all relevant inputs, and transparently reporting data sources, data quality, and underlying assumptions. Two main limitations of the LCI have been identified in this review: (1) incomplete or inconsistent reporting, and (2) discrepancies in the relationships between the elementary processes.

The review identifies several levels of problems in inventory reporting. The most critical issue is the complete lack of reporting for parts or entire inventories in some studies, which severely undermines transparency [17,21,28,29,40]. While most papers do report inventory data, they systematically present static datasets—that is, fixed, computed, or aggregated values without dynamic relationships between parameters. This limits the adaptability of the studies and complicates efforts to update or refine them. In addition, units of measurement vary across inventories. For example, stack manufacturing data may be reported per kW of stack, per m^2 of stack, or per unit of stack. However, the parameters required to convert between these units are often not provided, making it difficult to reconcile datasets and ultimately limiting comparability.

A second limitation lies in the inconsistent definition of key performance parameters—particularly system efficiency and system size. A variety of efficiency conventions exist: stack-limited or system efficiencies [24,42,48]; LHV-based[12,24,46,49], HHV-based[5,50] or thermoneutral-based efficiencies[51,52]; beginning of life or average efficiencies[15,45,53]. Similarly, the system capacity can be defined and compared in terms of electrical power [13,18,46] or hydrogen flowrate [19,20,42]. This diversity leads to misunderstandings and reveals a lack of clarity regarding what exactly is being assessed and how key parameters are interrelated. This underscores the need for more explicit definition of efficiency or capacity depending on the context.

The third limitation of the inventory lies in its dependency on specific technology capacity and technology readiness levels (TRLs). Comparison between systems is only relevant when the TRL and the capacity of the system are equivalent [10]. Yet, as FC&EL are still emerging technologies, their maturity and size are varying from one technology family to another [13]. To improve comparability across studies, there is a need for robust up-sizing (i.e., estimating the impacts of larger system configurations) and up-scaling (i.e., modeling future improvements in environmental performance) methodologies. As for now, up-sizing of FC & EL systems for LCA draws on economic empirical correlations [18,26], but these rely on cost-based relationships that are not necessarily representative of environmental dynamics, as economies of scale do not directly translate to environmental benefits. Up-scaling is commonly addressed by building prospective datasets based on expert judgment or field targets [10,14,42,43,45]. However, the lack of transparent reporting in many studies makes it difficult to distinguish between empirical and prospective datasets [10], ultimately leading to the creation of inconsistent inventories that combine empirical stack data with prospective operational performances [13,16,20,24].

2 – Methodological requirements derived from intended objectives of the LCA

In addition to addressing these challenges, a unified framework must also meet the specific requirements of each intended goal to ensure its applicability across all contexts. According to ISO, the intended goal of an LCA defines the purpose of the study. As outlined in the introduction, the main goals of LCAs applied to fuel cells and electrolysers (FC&EL) include: (i) comparing FC&EL technologies with conventional or alternative systems providing equivalent functions, (ii) benchmarking different FC&EL families, and (iii) supporting the eco-design of FC&EL systems. The following section details the methodological requirements derived from each intended objectives.

First, comparing FC&EL technologies with alternative systems providing equivalent functions requires a consistent system scope across technologies to ensure a proper supply chain-to-supply chain comparison. For this reason, functional units that reflect the final service delivered by hydrogen are required for this intended goal.

Second, comparing different families of FC&EL technologies requires consistent LCA modeling. This means that the system boundaries should be identical across all FC&EL families, including supply chain, system components and stack functional layers. A common inventory modeling with aligned assumptions for data collection and preparation is also required.

Third, for eco-design purposes, high-detailed inventories are essential. They provide greater precision and transparency, and they support sensitivity and contribution analyses needed to identify system hotspots and design levers. However, for other intended goals, highly detailed datasets are often avoided, as aggregated inventories are less time-consuming to compile and offer useful simplifications that enhance usability—particularly for broader-scale assessments and non-expert audiences. These divergent interests explain the variability in the level of detail observed across the literature. Stack manufacturing may rely on a generic model taken from LCA databases such as ecoinvent [18,25,26,29,33], static inventories at the stack level [14,19,22,24,46], layer level [13,27,35–37,39,43] or parametrized inventories [15,16,20,42]. Similarly, the BoP equipment is modeled with varying granularity—from aggregated material quantities [24,39,43,46] to detailed representations [15,18,27,36]. The key challenge lies in establishing granular LCI modeling for FC&EL systems that can accommodate different levels of detail, enabling inventories designed for eco-design to be meaningfully aggregated and compared with those developed for other purposes.

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