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LIFE CYCLE ASSESSMENT OF HYDROGEN PRODUCTION PATHWAYS IN CANADA

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Executive Summary

Canada has the potential to produce hydrogen as part of the clean fuel transition of its existing energy sector to a low-carbon economy, commitment that will support reaching net-zero emissions goal by 2050. Domestic hydrogen production is leveraged by the availability of diverse energy sources from fossil fuels to renewable electricity. Canada has the one of the cleanest electricity systems in the world with over 83% of electricity from non-emitting sources. Additionally, production of low-carbon hydrogen has the potential to be internationally traded. However, it is necessary to define and measure the carbon intensities of potential hydrogen production pathways in Canada in order to define low-carbon hydrogen in future standards. It is within this context that the National Research Council Canada (NRC), through its Advanced Clean Energy Program, has undertaken the development of a Life Cycle Assessment of Hydrogen Production Pathways in Canada Study, with support of the Natural Resources Canada (NRCan)'s Office of Energy Research and Development (OERD) and collaborators CanmetENERGY in Devon (CE-D), and CanmetENERGY in Varennes (CE-V) of NRCan, which have joined their efforts and expertise to provide hydrogen production process simulation results to complete the current study.

The purpose of this study is to develop a detailed and complete methodology based on a life cycle assessment (LCA) approach to assess different carbon intensities of hydrogen production in order to provide a consistent and verifiable greenhouse gases (GHG) estimation, including definition of system boundaries and building life cycle inventories for a Canadian context. Additionally, this report provides results of performing the proposed LCA-based methodological framework for two hydrogen production pathways in a Canadian context using steam methane reforming with natural gas and without carbon capture and alkaline electrolysis using grid electricity.

After performing a scoping review of relevant hydrogen LCA peer-reviewed studies, critical life cycle assessment methodological options were identified for harmonizing LCA of hydrogen production frameworks.

Based on current life cycle assessment normative, a methodological framework is developed to quantify carbon intensities of hydrogen production. LCA methodological choices such as definition of functional unit, system boundaries, and life cycle inventory criteria are aligned to relevant and current low-carbon intensity hydrogen standards. The LCA-based methodology is an attributional LCA, with the system boundaries being to the point of hydrogen production ('well-to-gate' approach). The life cycle inventory data for the foreground system comes from modelling and simulation results of the processes selected in this study.

A life cycle assessment was conducted to the steam methane reforming as baseline pathway and the alkaline electrolysis pathway. Life cycle GHG emissions results show that the baseline hydrogen pathway presents a wide range of improvement in comparison to an estimated low-carbon hydrogen threshold. Electrolysis pathway shows its carbon intensities depend on the share of renewable energy sources used to generate electricity as feedstock in the electrolysis process.

Further LCAs for the remaining hydrogen pathways in a Canadian context will be performed and results will be published in a new report.

It is important to note that the accuracy and completeness of the life cycle inventory data could be improved with primary data from current industry, hence it is recommended that the LCA results in the present report may be revised with use cases from current hydrogen projects developed in a Canadian context.

Additional recommended steps, include start a wide consultation process with stakeholders to revise life cycle GHG emissions estimates and to set the final carbon intensities threshold(s).

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Life Cycle Assessment of Hydrogen Production Pathways in Canada

1 Introduction

Hydrogen is a promising energy carrier that can replace fossil fuels in power and heat generation and transportation, with the potential to drastically reduce local pollution and greenhouse gases (GHG) emissions. Canada's hydrogen production potential offers vast economic opportunities across the country. Potential clean energy technologies to produce hydrogen are electrolysis, coined "green" hydrogen considering that 82% of Canada's electricity supply comes from either renewable or low-GHG-emitting sources, and steam-methane reforming (SMR) with carbon capture, coined "blue" hydrogen, offers a unique opportunity to leverage Canada's natural gas reserves to produce low-carbon energy. Additionally, Canada has vast biomass feedstock reserves which are technically feasible feedstock for renewable fuel production. Biomass gasification, a stable, thermochemical technology to convert biomass (forest, agricultural waste, and dry organic waste) into hydrogen and other gaseous products, is considered both renewable and carbon-neutral. When coupled with carbon capture and storage, the process becomes carbon-negative. Similarly, hydrogen production via SMR of bio-methane is a promising pathway and emission intensity is one of the lowest carbon intensities among all the different hydrogen production pathways. Bio-methane, which is a natural gas substitute to provide a renewable source of hydrogen production, is produced by anaerobic digestion processes of organic biomass feedstock (food waste, sewage and animal waste).

Several studies have considered the application of life cycle assessment (LCA) as an important and useful methodological option to quantify among others, the environmental impacts, the GHG emissions associated with hydrogen production, and thus it could facilitate a low-carbon hydrogen market through guarantee or certification of origin scheme.

This study aims to develop a detailed and complete LCA framework to assess different carbon intensities of hydrogen production in order to provide a consistent and verifiable GHG estimation, including definition of system boundaries and building life cycle inventories for a Canadian context. A preliminary life cycle assessment (LCA) is perform for two hydrogen production pathways in a Canadian context using the newly developed framework, steam methane reforming with natural gas and without carbon capture and alkaline electrolysis using grid electricity.

2 Background

From September 2021 to March 2022, the Energy, Mining and Environment (EME) Research Centre of the National Research Council Canada (NRC-EME), CanmetENERGY Devon (CE-D), and CanmetENERGY Varennes (CE-V) of Natural Resources Canada (NRCan) have joined their efforts and expertise to complete the project "LCA of Hydrogen Production Pathways in Canada, under the NRCan's OERD's program in the area of hydrogen codes and standards. In collaboration with CE-D and CE-V research teams, it was possible to model and simulate SMR of natural gas (without carbon capture) and alkaline electrolysis hydrogen production processes to generate critical input data to perform preliminary quantification of life cycle GHG emissions of these pathways.

This project is also well aligned with NRC's climate change strategy to provide environmental assessment of hydrogen production processes as part of a clean energy supply chain analysis, as envisioned by the NRC's Advanced Clean Energy (ACE) Program. Overall, this project could leverage collaboration with other federal department collaborators to access high-quality data, conduct detailed mass-energy balance analysis, and obtain feedbacks on the framework and results.

3 Objectives

The objectives to be pursued through this project are as follows:

i. Complete a comprehensive methodological framework to quantify the carbon intensities of hydrogen production pathways.

ii. Estimate hydrogen carbon intensities in a Canadian context of selected pathways to support National standard for quantification of life cycle GHG emissions of hydrogen production pathways, and certification schemes in Canada based on classification of hydrogen production intensities (a threshold for GHG emissions).

iii. Develop and implement a Canadian life cycle inventory (LCI) database of hydrogen production pathways. This LCI database will allow the interoperability of individual datasets to create LCI models for hydrogen production. The LCI data quality will be evaluated to ensure consistency within its data pool. This LCI database will be publicly accessible via a web server.

4 Scoping Review

A scoping review type is conducted as a way of mapping of the existing literature on the life cycle assessment of hydrogen production, identifying research gaps, and summarising the approaches used to develop LCA of hydrogen production and the relevant LCA's elements suggested for harmonizing LCA of hydrogen production frameworks (Arksey, 2005; Munn et al., 2018).

To complete this scoping review, five main steps are completed as follows[1]:

i. **Identify** – the main research field to be explored is the LCA approach to quantify carbon intensities of hydrogen production.
ii. **Find** – locate relevant studies using exploratory search – peer-reviewed publications, conference proceedings, public reports.
iii. **Select** – choose studies using a predetermined criteria (exclude studies in other languages than English, type of study different to LCA, and studies with more than 10 years of publication date.
iv. **Map**– organize the data from relevant studies selected in a tabular format and statistical analysis.
v. **Summarize** – summarize and report the results.

The key questions to cover in this scoping review are:

I. What is known from the existing literature about life cycle assessment methodologies to quantify GHG emissions of hydrogen production pathways?
II. How these methodologies are used to develop certifications of carbon intensities of hydrogen production?

This review's focus is on life cycle assessments studies of current commercial and emerging hydrogen production pathways relevant to Canada with a Technology Readiness Level (TRL) of 6 and above. In addition, it will include a review of international guarantee of origin/certifications of hydrogen.

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[1] https://libguides.lib.umanitoba.ca/reviewtypes/scoping

4.1 Selection of relevant studies

Two peer-reviewed searches using SCOPUS were conducted for each of the two questions, one to find global results for the past four years (89 publications), and another for Canada only in the past 10 years (14 publications). Each search was cross-checked for articles mentioning certification of origin of hydrogen, and none were identified.

In the first scan of the 103 peer-reviewed articles, 14 were excluded because it was either in Chinese or not accessible. In the second scan of the 89 remaining articles, 10 were excluded because these were focused on emerging technologies, ammonia production or fuel cell vehicles and not relevant to hydrogen production LCA studies, or with limited or outdated data. As a result, 79 peer-reviewed articles related to LCA of hydrogen production were selected to be analyzed in a tabular format.

Additionally, articles were collected from organisations working in the field such as the International Partnership for Hydrogen and Fuel Cells in the Economy (IPHE), the Hydrogen Council, the International Energy Agency (IEA), and the International Reference Life Cycle Data System (ILCD) as an initiative developed by Joint Research Centre (JRC) and the Directorate-General Environment (DG ENV) of the European Commission (EC).

4.2 Results

4.2.1 Review of LCA studies to quantify GHG emissions of hydrogen production pathways

Since life cycle assessment is a well-known and defined methodology to assess the potential environmental impacts of a product or a service, LCA and hydrogen are the keywords in the literature search performed to review and analyze publications related to GHG emissions quantification methodologies for hydrogen production pathways.

A review of methodological options of LCA studies of hydrogen value chain was performed. As result of a scanning procedure, 89 peer-reviewed studies published until 2021, from which 215 cases of hydrogen production LCAs were found. Figure 4-1 illustrates the share of LCAs studies for hydrogen production classified per technology category, where thermochemical, electrochemical, and biological technology categories represent 49%, 48%, and 3%, respectively. Among hydrogen technologies under review, the technologies with more occurrences are illustrated in Figure 4-2, where steam methane reforming (SMR) represents 31% of all the case studies, meanwhile electrolysis using energy sources as wind, solar PV, and grid electricity represent 14%, 10%, and 8%, respectively. Biomass gasification represents 9% of all hydrogen LCA's studies reviewed.

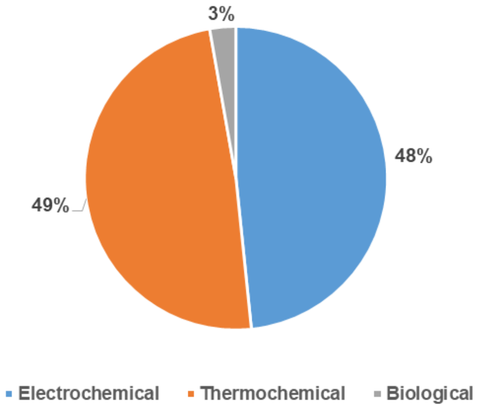

Figure 4-1: Life cycle assessment studies for hydrogen production per technology category

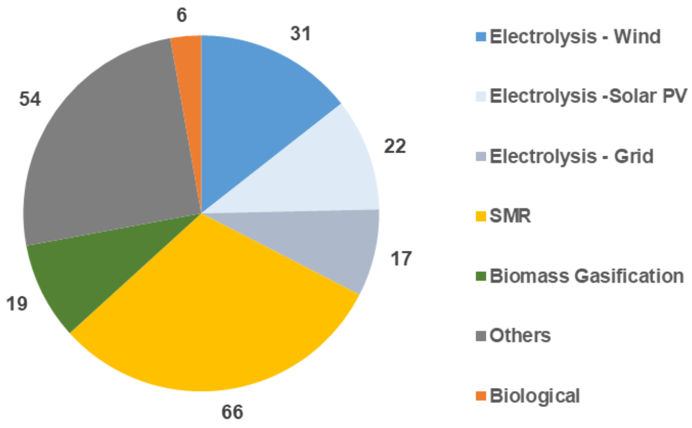

Figure 4-2: Number of LCAs case studies per specific hydrogen technology

To analyze the LCA methodologies used in the existing publications related to hydrogen production, further careful selection was made among those 89 peer-reviewed literatures. First of all, all review papers and those which are not very relevant to the global warming potential (GWP) impact studies were filtered out. In addition, the publications with similar studies, though with different emphasis, from the same research group were deemed as duplicate and only one of them was kept. Furthermore, those with hydrogen as a feedstock and without providing LCI data related to hydrogen production, were removed from the list as well. As a result, there are total of 40 publications remaining in the final list, which were used for the statistical analysis of LCA methodologies. The list of 40 publications being reviewed is provided in Appendix 9.1.

Regarding the geographical coverage of these hydrogen production LCA studies, 87% of the total 40 studies provide specific geographical locations, as shown in Figure 4-3. More than 70% present results are related to the European or the North America regions, with roughly equivalent distribution between these two. Within North America region, the number of studies for Canada is less than that for USA (15% vs. 20%).

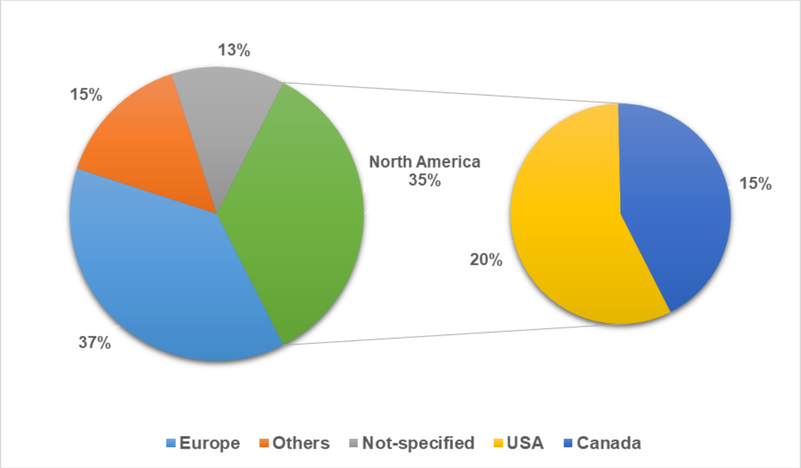

Figure 4-3: Geographical distribution of literatures reviewed for LCA GHG studies of hydrogen productions

Most of the LCA studies of hydrogen production along its supply chain are comparative but performed using different methodological options. Harmonization of common practices for life cycle assessment of hydrogen production is proposed in several studies (Iribarren, 2018; Antonio Valente, Iribarren, & Dufour, 2016, 2017; A. Valente, D. Iribarren, & J. Dufour, 2020; Antonio Valente, Iribarren, & Dufour, 2021; A. Valente, Iribarren, Galvez-

Martos, & Dufour, 2019), focusing on four relevant aspects covered by international standards such as ISO (2006b) and ISO (2018): (i) attributional approach, (ii) functional unit, (iii) system boundaries, and (iv) multifunctionality approach. Table 4-1 indicates the level of agreement of the 40 publications related to these key LCA methodological options.

Table 4-1: Level of agreement of key LCA methodological options

Life cycle assessment stage	Element	Level of agreement
Hydrogen product system information	Purity >= 99.9%	Very high
	Pressure > 3 Mpa	Low
Goal and scope definition	Unambiguously define the goal of the study	Very high
	Cradle-to-gate system boundary	High
	Compression process included in the system boundary	Low
	Use energy (MJ H2) of produced hydrogen as the functional unit	Low
	Use mass (kg H2) of produced hydrogen as the functional unit	High
	Use the ISO system expansion allocation for solving multifunctional processes	Low
	Use the ISO physical allocation for solving multifunctional processes	Very high
	Processes rated to embedded emissions from construction, manufacturing of capital goods excluded from system boundary	Very low
Life cycle inventory analysis	Define data quality requirements according ISO standards	Very low
	Use primary data for the foreground processes	Low
	Fill data gaps with secondary data	Very high
Life cycle impact assessment	Use the Global Warming Potential impact category	Very high
	Use IPCC as impact method	Low

Level of agreement:
Very low<=10% of the case studies
Low 11-40%
Intermediate 41-60%
High 61-90%
Very high >= 91%
Based on 40 publications between the years 2017-2021 and extended to 2010 for geographical coverage of Canada.

Nearly all of the 40 studies look at hydrogen produced at a very high purity (>=99%), but the pressure condition at final stage could vary with 18% of the studies specified as > 3 MPa. On another hand, very few papers provided the temperature condition of the final hydrogen product. Regarding the system boundary, all the publications in the list clearly stated if it is cradle-to-gate or cradle-to-grave (very few cases used the term of Wheel-to-grave instead of cradle-to-grave), among which the studies using cradle-to-gate system boundary take up 80%. In terms of functional unit, 80% vs. 12% used mass (1 kg) and energy (1 MJ/GJ/MW) of hydrogen, respectively. For the life cycle inventory data of the hydrogen production technologies, there are 35% of them using partial primary data for the foreground processes, which can be from real plants, process simulations, experimental measurements, or other consulting results. The other data gaps were all filled up with secondary data which were obtained from other publications and/or existing databases. Regarding the life cycle impact assessment, all studies in the list use the GWP impact category since this is used as one literature filtering criteria, and 70% of them analyzed at least one more other impact factor as well. For the detail impact method, not all studies provided this information (15% not specified), and the listed methods vary a lot. The most commonly used impact methods include CML (17%), IPCC (20%), ILCD (15%) and ReCiPe (23 %), indicating no dramatic preference of one over the other although ReCiPe and IPCC have a relatively high percentage.

Whenever the multifunctional processes were considered (the total number of such studies in the analysis is low (1/8)), various methods were applied, including substitution, system expansion, and physical allocation based on energy content, mass or market value. There is no clear priority of one method over another observed, which may be due to the limited number of related publications, or the adoption of a method for multifuctionality really depends on the specific application cases and detail considerations. At last, it is noted that there is no literature identified here that performed the data quality analysis. Instead data uncertainty analysis was performed but in very few publications (2 out of 40) (Palmer, Roberts, Hoadley, Dargaville, & Honnery, 2021; Sadeghi, Ghandehariun, & Rosen, 2020a), using a risk analysis through Monte-Carlo simulation, to account for the uncertainty of data used in the inventory analysis.

4.2.2 Comparison of current international guarantee of origin (GO)/certifications of hydrogen

4.2.2.1 Hydrogen strategies

National hydrogen strategies and roadmaps reports from different countries are compiled and summarized as follows:

4.2.2.1.1 Australia

Australia's National Hydrogen Strategy sets a vision for a clean, innovative, safe and competitive hydrogen industry that benefits all Australians. It aims to position our industry as a major global player by 2030.

The hydrogen strategy:

- explores Australia's clean hydrogen potential;
- considers future scenarios with wide ranging growth possibilities;
- outlines an adaptive approach that equips Australia to scale up quickly;
- includes showcases from each state and territory;
- details the nationally coordinated actions involving governments, industry and communities.

Australia is a leading country in the Guarantee of Origin (GO) scheme. More information on Australia's GO scheme can be found in the discussion paper entitled A Hydrogen Guarantee of Origin scheme for Australia.

4.2.2.1.2 Canada

Hydrogen strategy for Canada was prepared by Natural Resources Canada in December 2020. It lays out an ambitious framework for actions that will cement hydrogen as a tool to achieve Canada's goal of net-zero emissions by 2050 and position Canada as a global, industrial leader of clean renewable fuels.

In addition to Canada's hydrogen roadmap, the provincial Government of British Columbia published its own roadmap, (BC, N.D.), to combat the effect of climate change and meet Paris agreement's emissions reduction targets. In (Zen, 2019), a hydrogen study is conducted to identify roles hydrogen can play by 2030 and 2050.

The provincial Government of Alberta published also a hydrogen roadmap (Alberta, 2021), which provides an action plan focus on growth and commercialization of hydrogen in the Alberta's' energy economy.

4.2.2.1.3 European Union

Two relevant reports were found. Both of them are summarized below:

4.2.2.1.3.1 Hydrogen Roadmap Europe – A Sustainable Pathway for the European Energy Transition

The report describes an ambitious scenario for hydrogen deployment in the EU to achieve the 2-degree target. This scenario is based on the perspective of the global Hydrogen Council, input from Hydrogen Europe (representing the European hydrogen and fuel cells industry), and, more specifically, data from 17 member companies active in hydrogen and fuel cell technologies. As part of the Paris agreement, EU member states have committed to achieving the 2-degree scenario and making efforts towards achieving a 1.5-degree scenario (EU, 2019). Both scenarios refer to decreasing the global warming "well below 2 degrees Celsius above preindustrial levels, and to pursue efforts to limit the temperature increase even further to 1.5 degrees Celsius."(EU, 2019)

4.2.2.1.3.2 Communication from The Commission to The European Parliament, The Council, The European Economic and Social Committee and the Committee of The Regions – A hydrogen strategy for a climate-neutral Europe (EU, 2020)

This report outlines:

i. Why Europe needs a strategic road map for hydrogen;

ii. A roadmap for the EU;
iii. An investment agenda for the EU;
iv. Boosting demand and scaling production;
v. Designing a framework for hydrogen infrastructure and market rules;
vi. Promoting research and innovation hydrogen technologies;
vii. The international dimension;
viii. Key actions.

4.2.2.1.4 Germany

The National Hydrogen Strategy was published by the Federal Ministry for Economic Affairs and Energy in June 2020 (Germany, 2020). It is an action plan that outlines:

i. the goals and ambitions of Germany in regard to hydrogen,
ii. the status quo, fields of action and markets of the future,
iii. the governance for the National Hydrogen Strategy,
iv. the steps necessary for the National Hydrogen Strategy to succeed.

The report does not refer to efforts regarding guarantee of origin scheme, carbon intensity pathways or measurement of carbon intensities.

4.2.2.1.5 Japan

The Strategic Road Map for Hydrogen and Fuel Cells - Industry-academia-government action plan to realize a “Hydrogen Society” was published on March 12, 2019. This road map provides Japan’s policy direction for realizing a hydrogen-based society as an important element of the Basic Hydrogen Strategy (Japan, 2019).

4.2.2.1.6 UK

The UK Hydrogen Strategy was published in August 2021. This report makes the case for low carbon hydrogen and outlines the approach to developing the UK hydrogen economy. It continues to explain how economic opportunities will be secured across the UK that can come from a thriving hydrogen economy. The report also shows how the UK is working with other leading hydrogen nations to drive global leadership on the development of low carbon hydrogen to support the world’s transition to net zero. The report concludes with how progress will be tracked (BEIS, 2021b). Additionally, the report entitled Options for a UK low carbon hydrogen standard was published in May 2021 to identify and compare options for a UK standard that defines low carbon hydrogen (BEIS, 2021).

4.2.2.1.7 US

4.2.2.1.7.1 Roadmap to a US Hydrogen Economy

A coalition of major oil & gas, power, automotive, fuel cell, and hydrogen companies have come together to develop a Road Map to a US Hydrogen Economy. The Fuel Cell and Hydrogen Energy Association, (FCHEA) which represents the leading companies and organizations that are advancing innovative, clean, safe, and reliable energy technologies, coordinated the group and managed the process (FCHEA, 2020).

This report describes a road map for transitioning to a hydrogen economy in which hydrogen becomes a mainstream fuel option. It was developed to put forward a concrete proposal for various sectors and applications that may be developed and deployed in the coming years. It provides milestones for deployment and leverages domestic strengths to deliver on the vision set out in the first half of this report. This report aims to serve as a reference document for policymakers and industry. The road map is organized into four key phases: 2020 to 2022, 2023 to 2025, 2026 to 2030, and post-2030. Each phase has specific milestones for the deployment of hydrogen across applications. Each phase also describes the key enablers required, categorized as (i) policy enablers and (ii) hydrogen supply and end-use equipment enablers. Policy enablers are needed initially to create the right incentives to enable the private sector to invest in and develop the hydrogen market.

4.2.2.1.7.2 Hydrogen Strategy – Enabling a low-carbon economy

This document summarizes current hydrogen technologies and communicates the U.S. Department of Energy, Office of Fossil Energy's (FE's) strategic plan to accelerate research, development and deployment of hydrogen technologies in the United States. It also describes ongoing FE hydrogen-related research and development. Hydrogen produced from fossil fuels is a versatile energy carrier and can play an important role in a transition to low-carbon economy (DOE, 2020).

4.2.2.2 Guarantee of origin (GO)/certifications of hydrogen

A Guarantee of Origin (GO) is an electronic document that guarantees and provides information to end users on the origin of a product (CertifHy, N.D). Overall guarantee of origin (GO) is based on a "book and claim" approach whereas certifications of hydrogen present more extensive requirements (BEIS, 2021).

Europe is a region that is leading the development of hydrogen guarantee of origin and certifications schemes. One example is the certification system CertifHy, which has launched a European GO scheme.

CertifHy relies on Guarantees of Origin for certifying the origin of the hydrogen feedstock. CertifHy is developed by a consortium led with Hinicio, Ludwig Bölkow Systemtechnik (LBST), Grexel, TNO and TÜV SÜD and financed by the Fuel Cell and Hydrogen Joint Undertaking. CertifHy is following extensive consultations with 900+ members of the CertifHy Stakeholder Platform and its topical Working Groups that bring together European stakeholders with an interest in Green and Low Carbon hydrogen. Between 2014 and 2016, the CertifHy project (phase 1) developed an EU-wide Green and Low Carbon Guarantee of Origin (GO) Scheme including a definition for Green and Low Carbon hydrogen and a roadmap with concrete steps for the implementation of an EU-wide GO scheme. The follow-up (CertifHy project phase 2), which ran between October 2017 and March 2019, built on the momentum and served as a catalyst for implementing an EU-wide GO scheme for Green and Low Carbon hydrogen.

CertifHy enters into phase 3 to build a H_2 GO market as well as a H_2 certification scheme for the European Commission - Renewable Energy Directive II (RED II)[2]. The RED II defines a series of sustainability and GHG emission criteria that bio liquids used in transport must comply with to be counted towards the overall 14% target and to be eligible for financial support by public authorities. Some of these criteria are the same as in the original RED, while others are new or reformulated. In particular, the RED II introduces sustainability for forestry feedstock as well as GHG criteria for solid and gaseous biomass fuels.

The CertifHy Scheme document governs the CertifHy Scheme – a European Certification Scheme for hydrogen fulfilling specific criteria. At this stage, this document covers Guarantees of Origin, and the framework leaves room for additional purposes. CertifHy published a roadmap entitled Taking CertifHy to the next level – Roadmap for building a dual hydrogen certification infrastructure for Guarantees of Origin and for Certification of renewable hydrogen in transport. The roadmap was last updated on March 19, 2019.

A summary of a comparison between six GO/ certifications initiative and/or proposed hydrogen standards is provided in Table 4-2. These six case studies are:

I. CertifHy – voluntary Guarantee of Origin scheme within the European Union (EU)
II. AFHYPAC - voluntary Guarantee of Origin scheme by French Association for Hydrogen & Fuel Cells
III. LCFS - Low Carbon Fuel Standard in California, USA

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[2] https://joint-research-centre.ec.europa.eu/welcome-jec-website/reference-regulatory-framework/renewable-energy-recast-2030-red-ii_en

IV. TÜV SÜD – voluntary renewable hydrogen standard in Germany. Active certification scheme with two options GO at point of hydrogen production or point of use certification with mass balancing approach.
V. BEIS- UK Low Carbon Hydrogen standard (consultation process only)
VI. IPHE - International Partnership for Hydrogen and Fuel Cells in the Economy, Hydrogen Production Analysis (H_2PA) Task Force5.
VII. Australian Government Scheme – Proposed certification scheme

Table 4-2: Comparison of worldwide current active or proposed hydrogen certification schemes and/or national strategies, adapted from White et al. (2021)

Certification scheme/ Strategy	Jurisdiction	Functional unit	Allocation	Threshold	System boundary					
					Emissions embedded in capital goods	Feedstock	Production	Conversion	Transport	Use
Certifhy (Pilot GO)	EU wide	$kgCO_{2e}/MJ\ H_{2\ LHV}$	Energy content	60% lower GHG than reference grey hydrogen (SMR-NG)	Excluded (align with low carbon fuel standards and REDII Europe	Yes	Yes	No	No	No
AFHYPAC (proposed GO)	France	Not specified		100% Renewable – no baseline	Excluded	Yes	Yes	No	No	No
LCFS (active LCA for transport)	California	$gCO_{2e}/MJ\ H_2$	Mixed. Mostly by energy, or system expansion where non-energy outputs	30% lower GHG, 50% lower NOx for fuel cell vehicles	Excluded	Yes	Yes	Yes	Yes	Yes
TUV SUD (active certification)	Germany, Europe	$kgCO_{2e}/MJ\ H_{2\ LHV}$	Energy-based and market-value based allocation	35-75% lower GHG than reference grey hydrogen (SMR-NG)	Excluded	Yes	Yes	Yes	Yes	No
BEIS-UK Low carbon hydrogen standard (consultation process only)	UK	$kgCO_{2e}/MJ\ H_{2\ LHV}$	Energy content	Energy content	Options: a. Excluded b. Included for H_2 production only c. Included for all supply chain equipment	Yes	Yes	No	No	No
IPHE (proposed GHG emissions methodology)	Worldwide	$kgCO_{2e}/MJ\ H_{2\ LHV}$	Still on discussion	None	Excluded	Yes	Yes	No	No	No
Australian Government (proposed certification scheme)	Australia	$kgCO_{2e}/kg\ H_{2\ LHV}$	System expansion and energy content	A materiality threshold of between 2.5 and 5% in total prior to carbon capture.	Excluded	Yes	Yes	No	No	No

AFHYPAC: French Association for Hydrogen & Fuel Cells
LCFS: Low carbon fuel standard
BEIS: Department for Business, Industry & Industrial Strategy

The common approach in the different GOs and certifications schemes is the definition of the hydrogen system boundary for carbon accounting using a process-based approach. Figure 4-4 illustrates the carbon accounting system boundaries for different hydrogen GO/certification schemes initiatives. Although a "well-to-tank" or "well-to-wheel" boundaries cover the downstream supply chain to the point of use or at the end of the application use, "well-to-gate" is the most common system boundary for hydrogen carbon accounting, which cover the entire upstream supply chain to the exit gate at point of production. In a “well-to-gate” approach or at point of production boundary, the purity and pressure are requirements to be complied for certification, very similar to a GO approach that CertifHy relies on. Additionally, “well-to-gate” approach present the risk to potentially omit large amount of emissions of downstream distribution GHG emissions that some hydrogen pathways may present, however that implies higher compliance costs such as data gathering, LCA calculations, third party auditing costs and other fees.

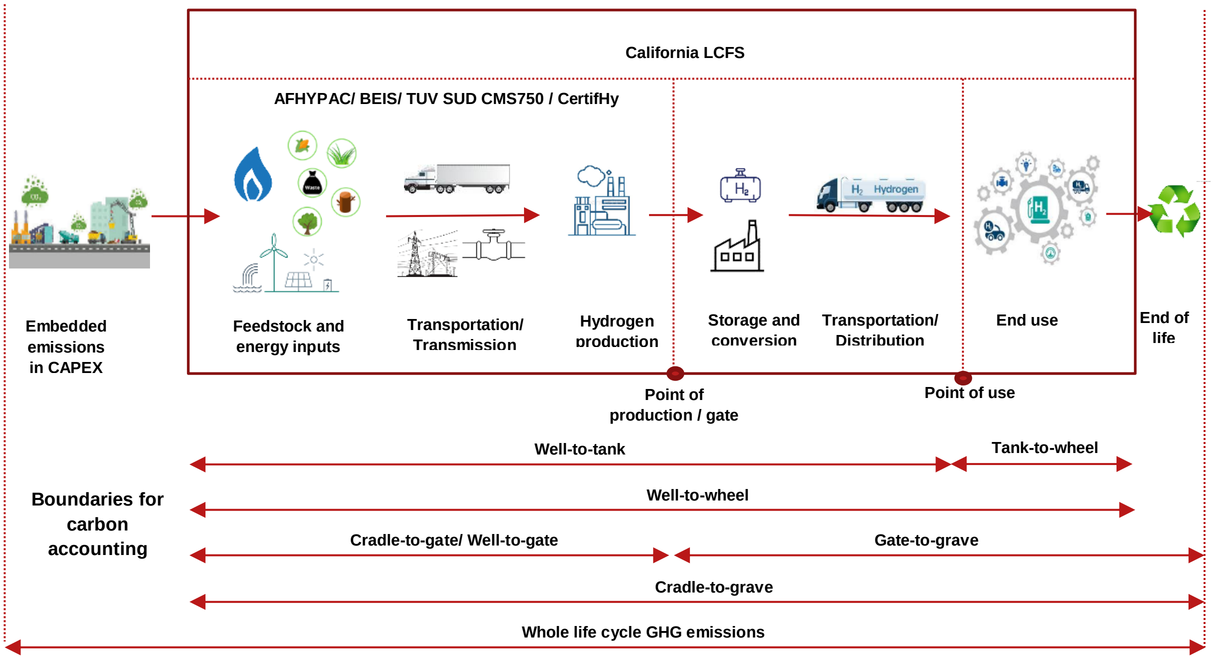


Figure 4-4: Carbon accounting system boundaries for different hydrogen GO/certification schemes initiatives, adapted from Velazquez Abad and Dodds (2020)

5 Methodology

5.1 Methodological framework for GHG emissions quantification of hydrogen production pathways

This proposed framework provides methods and procedures to quantify CO_{2e} intensities of different hydrogen production pathways, which in turn use a variety of feedstock sources. In a Canadian context, a quantification of GHG emissions of relevant hydrogen production pathways may provide a guidance on threshold values be proposed to facilitate a hydrogen certification scheme and/or develop a national standard of GHG emissions quantification methodology.

5.1.1 General principles

The methodology used to develop this greenhouse gases quantification model for hydrogen production pathways follows the life cycle assessment (LCA) approach, a well-established methodology for the comprehensive evaluation of the potential environmental impacts of product systems. LCA is also an environmental management technique that evaluate in a systematic way the environmental impacts of a product system throughout its life cycle (ISO, 2006a).

5.1.1.1 LCA normative references

This methodology for hydrogen production pathways and carbon intensities quantification follows the principles, requirements, and guidelines defined by the International Organization for Standardization (ISO) standards, *"Environmental management — Life cycle assessment — Principles and framework"* (ISO 14040:2006), *"Environmental management — Life cycle* assessment — *Requirements and guidelines"* (ISO 1444:2006/ Amendment 2:2020) and "Greenhouse gases — Carbon footprint of products — Requirements and guidelines for quantification" (ISO 14067:2018) as well as the 2004 GHG Protocol and the 2010 ILCD Handbook (ILCD, 2010a, 2010b; ISO, 2006a, 2006b, 2018, 2020; WRI, 2004). Figure 5-1 illustrates the life cycle assessment approach based on international standards, protocols and guidelines.

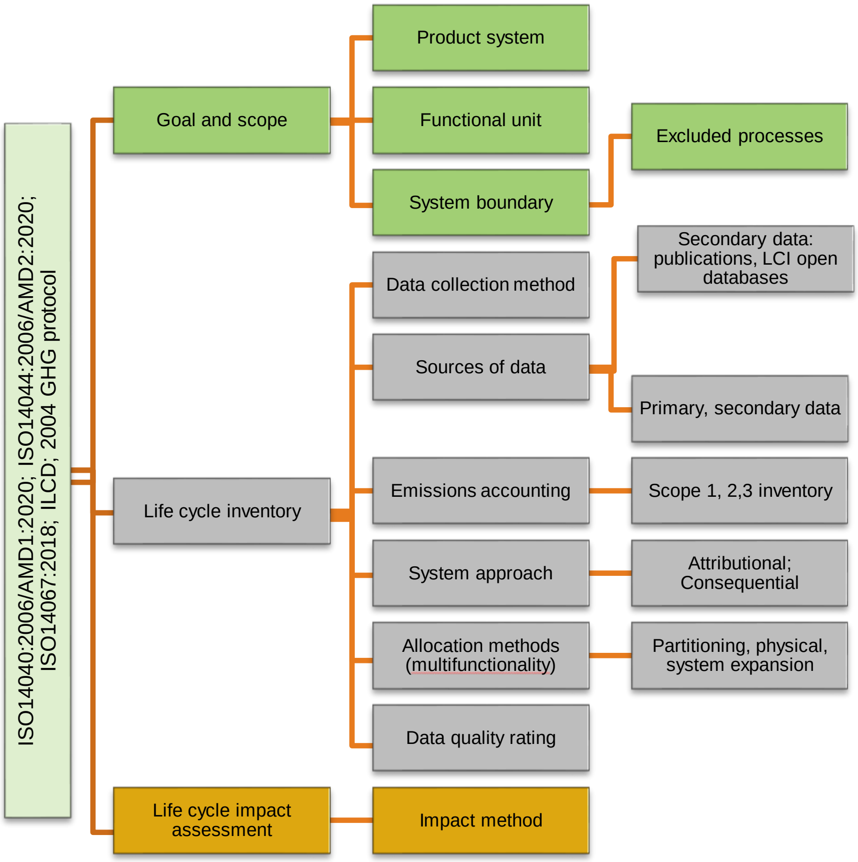


Figure 5-1: Life cycle assessment approach

5.1.1.2 Principles

The hydrogen LCA methodology to quantify GHGs is based on the principles of the normative ISO (2006a) and ISO (2018) being the main principles to take into account as follow:

5.1.1.2.1 Life cycle perspective.

The hydrogen LCA model and the quantification of carbon intensities are based on a life cycle approach which takes into account the entire life cycle of hydrogen production, including acquisition/extraction of raw material, feedstock production and transportation, hydrogen production, and hydrogen compression.

5.1.1.2.2 Relative approach and functional unit.

The carbon intensities calculation for hydrogen production pathways are based around a functional unit (FU) and the results are calculated relative to this FU.

5.1.1.2.3 Relevance.

The data collected are applicable and suitable to assess the GHG emissions and removals from the system under study.

5.1.1.2.4 Completeness.

All the GHG emissions and removals that provide a significant contribution to the carbon footprint of the product system under study are included. The level of significance is determined by the cut-off criteria.

5.1.1.2.5 Consistency.

The definition of the functional unit and system boundary are consistent with the goal of this LCA study. At the same time, the LCA approach is consistent among all the technologies evaluated in this study to allow for a valid comparison of GHG emissions between the different pathways for hydrogen production.

5.1.1.2.6 Transparency.

As in ISO 1467:2018, this LCA study considers a complete explanation of the methodology, including the assumptions related to definition of product system, functional unit, and system boundary. In the case of the hydrogen production process modelling and simulation, the operation condition assumptions, relevant issues, and estimates are explained and disclosed with data sources referenced. Data sources used in the life cycle inventory are also referenced.

5.1.1.3 Terminology

The terminology used in this document is presented in this section. These common terms and definitions are taken from ISO standards and GHG's protocols (ISO, 2006a, 2018; WRI, 2004) and adapted whenever is possible.

product system
collection of unit processes with elementary and product flows, performing one or more defined functions, and which models the life cycle of a product

[SOURCE: ISO 14040:2006]

functional unit
quantified performance of a product system for use as a reference unit

[SOURCE: ISO 14040:2006]

input
product, material or energy flow that enters a unit process
NOTE Products and materials include raw materials, intermediate products and co-products.

[SOURCE: ISO 14040:2006]

output
product, material or energy flow that leaves a unit process
NOTE Products and materials include raw materials, intermediate products, co-products and releases.

[SOURCE: ISO 14040:2006]

process
set of interrelated or interacting activities that transforms inputs into outputs

[ISO 9000:2005, definition 3.4.1 (without notes)]

[SOURCE: ISO 14040:2006]

unit process

smallest element considered in the life cycle inventory analysis for which input and output data are quantified

[SOURCE: ISO 14040:2006]

process energy
energy input required for operating the process or equipment within a unit process, excluding energy inputs for production and delivery of the energy itself

[SOURCE: ISO 14040:2006]

process emissions
Emissions generated from manufacturing processes

[SOURCE: 2004 GHG Protocol (Chapter 4, Appendix D)]

fugitive emissions
emissions that are not physically controlled but result from the intentional or unintentional releases of GHGs

[SOURCE: 2004 GHG protocol (Chapters 4, 6)]

co-product
any of two or more products coming from the same unit process or product system

[SOURCE: ISO 14040:2006]

product flow
products entering from or leaving to another product system

[SOURCE: ISO 14040:2006]

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

[SOURCE: ISO 14040:2006]

energy flow
input to or output from a unit process or product system, quantified in energy units
NOTE Energy flow that is an input can be called an energy input; energy flow that is an output can be called an energy output.

[SOURCE: ISO 14040:2006]

intermediate flow
product, material or energy flow occurring between unit processes of the product system being studied

[SOURCE: ISO 14040:2006]

reference flow
measure of the outputs from processes in a given product system required to fulfil the function expressed by the functional unit

[SOURCE: ISO 14040:2006]

feedstock energy
heat of combustion of a raw material input that is not used as an energy source to a product system, expressed in terms of higher heating value or lower heating value

NOTE Care is necessary to ensure that the energy content of raw materials is not counted twice.

[SOURCE: ISO 14040:2006]

raw material
primary or secondary material that is used to produce a product
NOTE Secondary material includes recycled material.

[SOURCE: ISO 14040:2006]

allocation
partitioning the input or output flows of a process or a product system between the product system under study and one or more other product systems

[SOURCE: ISO 14040:2006]

cut-off criteria
specification of the amount of material or energy flow or the level of significance of greenhouse gas emissions associated with unit processes or the product system to be excluded from a carbon footprint study

[SOURCE: ISO 14067:2018]]

system boundary
set of criteria specifying which unit processes are part of a product system under study
NOTE The term "system boundary" is not used in this International Standard in relation to LCIA.

[SOURCE: ISO 14040:2006]

Scope
Defines the operational boundaries in relation to indirect and direct GHG emissions

[SOURCE: 2004 GHG protocol (Chapter 4)]

Scope 1 Inventory
A reporting organization’s direct GHG emissions

[SOURCE: 2004 GHG protocol (Chapter 4)]

Scope 2 Inventory
A reporting organization’s emissions associated with the generation of electricity, heating/ cooling, or steam purchased for own consumption

[SOURCE: 2004 GHG protocol (Chapter 4)]

Scope 3 Inventory
A reporting organization’s indirect emissions other than those covered in scope 2

[SOURCE: 2004 GHG protocol (Chapter 4)]

data quality
characteristics of data that relate to their ability to satisfy stated requirements

[SOURCE: ISO 14040:2006]

primary data
quantified value of a process or an activity obtained from a direct measurement or a calculation based on direct measurements

Note 1 primary data need not necessarily originate from the product system under study because primary data might relate to a different but comparable product system to that being studied

Note 2: primary data can include greenhouse gas emission factors and/or greenhouse gas activity data

[SOURCE: ISO 14067:2018]

secondary data
data which do not fulfil the requirements for primary data

Note 1 secondary data can include data from databases and published literature, default emission factors from national inventories, calculated data, estimates or other representative data, validated by competent authorities

Note 2: secondary data can include data obtained from proxy processes or estimates.

[SOURCE: ISO 14067:2018]

site-specific data
primary data obtained within the product system

Note 1: all site-specific data are primary data but not all primary data are site-specific data because they may be obtained from a different product system

Note 2: site-specific data include greenhouse gas (GHG) emissions from GHG sources as well as GHG removals by GHG sinks for one specific unit process within a site

[SOURCE: ISO 14067:2018]

uncertainty analysis
systematic procedure to quantify the uncertainty introduced in the results of a life cycle inventory analysis due to the cumulative effects of model imprecision, input uncertainty and data variability
NOTE Either ranges or probability distributions are used to determine uncertainty in the results.

[SOURCE: ISO 14040:2006]

characterization factor
factor derived from a characterization model which is applied to convert an assigned life cycle inventory analysis result to the common unit of the category indicator
NOTE The common unit allows calculation of the category indicator result.

[SOURCE: ISO 14040:2006]

impact category
class representing environmental issues of concern to which life cycle inventory analysis results may be assigned

[SOURCE: ISO 14040:2006]

impact category indicator
quantifiable representation of an impact category.
NOTE The shorter expression "category indicator" is used in this International Standard for improved readability.

[SOURCE: ISO 14040:2006]

5.1.2 Proposed methodological framework

The hydrogen production LCA-based methodology for GHG emissions quantification proposed in this study is illustrated in Figure 5-2. This framework includes all the stages to account for and calculate the carbon footprint related to the different hydrogen production pathways in Canada. Starting with the goal and scope definition, setting up criteria to define the system boundary through building and modelling a consistent and transparent life cycle inventory to quantify carbon intensities (CIs) of hydrogen production. This methodology will be applied to different hydrogen production pathways in a Canadian context in order to classify these pathways by threshold of carbon intensities. In the context of hydrogen certification, international organizations attempt a classification of hydrogen production from non-low carbon and low carbon using a benchmark emissions intensity threshold.

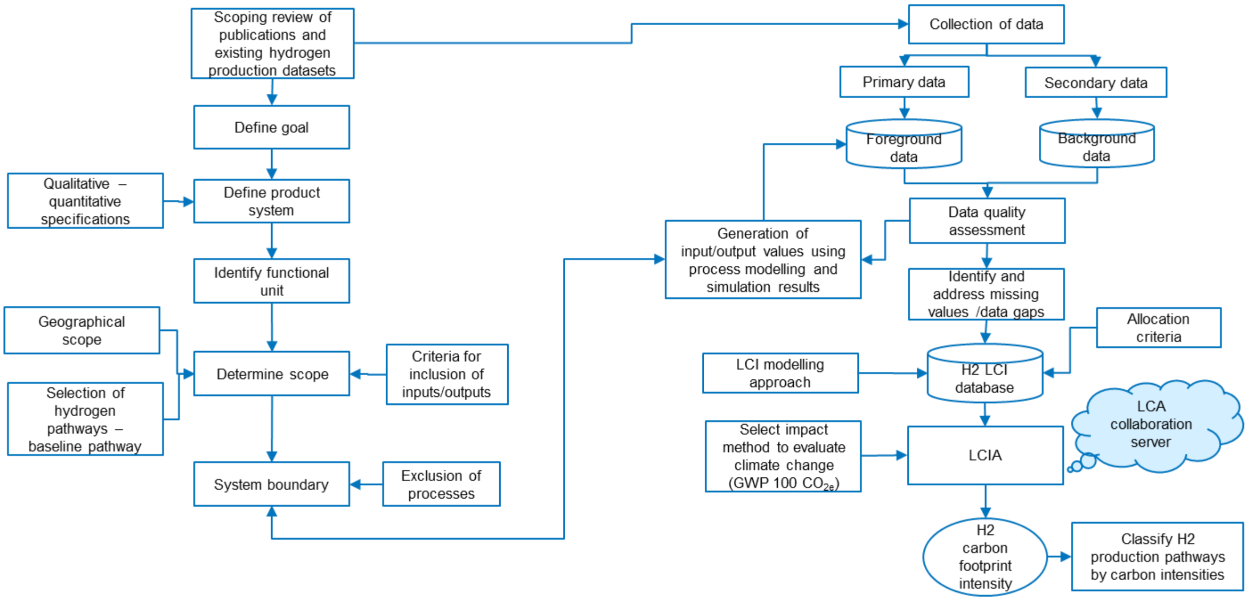


Figure 5-2: Hydrogen production LCA-based methodology framework

The following sections describe all the methods and procedures that comprise the LCA-based methodology for the quantification of GHG emissions of hydrogen production. The goal and scope will be defined as well as data collection methods, data quality evaluation procedures, the impact assessment method selected, and limitations of this study.

5.1.3 Goal and scope definition

5.1.3.1 Goal

The overall goal is to conduct a carbon footprint study, i.e. to calculate the potential contribution of hydrogen production to global warming (GWP) expressed in CO_{2e} by quantifying the GHG emissions along all the unit processes in conformity of ISO 14040:2006, 14044:2006, and 14067:2018 requirements. The goal of the LCA of hydrogen production pathways in Canada is to quantify the aggregated GHG emissions of the pathways selected and proposed carbon intensities threshold to certify low-carbon hydrogen in order to facilitate international trade of hydrogen by implementing hydrogen certification schemes and/or support the development of GHG emissions quantification methodology standards. Certification of embedded emissions will perform a strategic role in the future of hydrogen as a low-emission energy carrier.

Also, the life cycle inventory database for hydrogen production in Canada will be publicly available through a NRC-LCA Collaboration Server allowing for the life cycle carbon footprints calculation of hydrogen produced in Canada.

In order to compare the results of LCAs of different hydrogen production pathways, the assumptions and context of each study need to be equivalent by complying transparency requirements (IPHE, 2021; ISO, 2006b).

5.1.3.2 Scope

The scope of this LCA study will be consistent with the goal of the LCA for hydrogen production pathways (ISO, 2006b).

5.1.3.2.1 Product System

In the hydrogen LCA study, the function to be assessed is the production of hydrogen in gaseous state to be used in different applications in Canada.

The harmonized specifications of the product system at point of production are listed in Table 5-1 based on the IPHE's report and the scoping review of publications on hydrogen production LCA studies. The default pressure of 3 MPa is a common pressure value for the most steam methane reforming production pathway and a purity, industrial grade at gate greater or equal to 99% as minimum, however purity values of 99.9% or even 99.95% could be considered (IPHE, 2021). Related to the hydrogen energy content, despite the use of higher heating values (HHV) as hydrogen energy content in US and Canada to calculate carbon footprint, lower heating value (LHV) will be used as energy content of hydrogen to be aligned with current hydrogen certification schemes in other countries (CertifHy, 2019; IPHE, 2021).

It is required that all the hydrogen production pathways fulfil this product system specifications in this LCA study.

Table 5-1: Specifications of hydrogen product system at point of production (at gate)

Specifications	Reference values
State of hydrogen	Compressed gaseous
Purity, industrial grade	>= 99.9%
Default pressure	>= 3 Mpa
Temperature	25°C
Energy content, LHV	119.9 MJ/kg

5.1.3.2.2 Functional unit

As in ISO (2006b), the functional unit (FU) quantifies the function or performance of the product system and provides a measurable reference flow to which the input and output data is normalized. The FU must be specified accordingly to the goal and scope of this LCA study. The FU for hydrogen production systems should allow a complete identification of an amount of hydrogen with clear statement about energy content using the LHV (CertifHy, 2019).The quantitative aspect of the functional unit for this product system is expressed in a measured amount of mass (kg) to allow a valid comparison on a mass basis with other hydrogen production pathways.

The FU and reference flow are stated as ***"Production of 1 kg of compressed gaseous hydrogen (LHV) at a default pressure level greater than or equal to 3 Mpa and ambient temperature (25°C). The purity of industrial grade of hydrogen at gate greater or equal to 99.9%".***

The functional unit of 1 kg of hydrogen produced will be used for all the production pathways in selected Canadian provinces.

The carbon footprint (carbon intensity) is expressed in kilograms of carbon dioxide equivalents (kg CO_{2e}) per unit of mass of hydrogen produced in kilograms (kg).

5.1.3.2.3 Geographical scope

The hydrogen production LCA model is developed under a Canadian context considering the provinces that specific hydrogen production technologies have the potential to be developed.

Hydrogen production from fossil fuels with carbon capture is an alternative for clean hydrogen. The provinces with the highest natural gas reserves are Alberta, British Columbia, Saskatchewan, and the Atlantic Provinces, which are the best alternatives to produce hydrogen from fossil fuels (NRCan, 2020).

Hydrogen can also be produced from water via electrolysis using renewable sources, a hybrid alternative is hydrogen production using nuclear electricity at high temperatures. Provinces that have the greatest hydroelectric power production are Manitoba, Quebec, Newfoundland and Labrador, and British Columbia. Meanwhile, the provinces with highest number of wind facilities are Ontario, Quebec, and Alberta, while Ontario has 98% of solar installations in Canada. High temperature nuclear and electrolysis pathway can be potentially developed in the provinces of Ontario and New Brunswick (NRCan, 2020).

Most provinces in Canada have access to sustainable biomass as feedstock of waste-to energy processes, being British Columbia, Ontario, Alberta, Quebec and New Brunswick with the largest biomass capacity (NRCan, 2020).

5.1.3.2.4 Selection of pathways

The life cycle greenhouse gas emissions of these production pathways depend on the technology and energy source used (European-Commision, 2020).

This study of hydrogen LCA study aims to estimate life cycle GHG emissions intensities for a selection of hydrogen production pathways in a Canadian context. Based on the scoping review in section 4 and review of federal and provincial hydrogen strategies to achieve our goal of net-zero emissions by 2050 (Alberta, 2021; NRCan, 2020; Zen, 2019), the relevant hydrogen production pathways in Canada with a technological readiness level (TRL) >= 6 are identified in Figure 5-3.

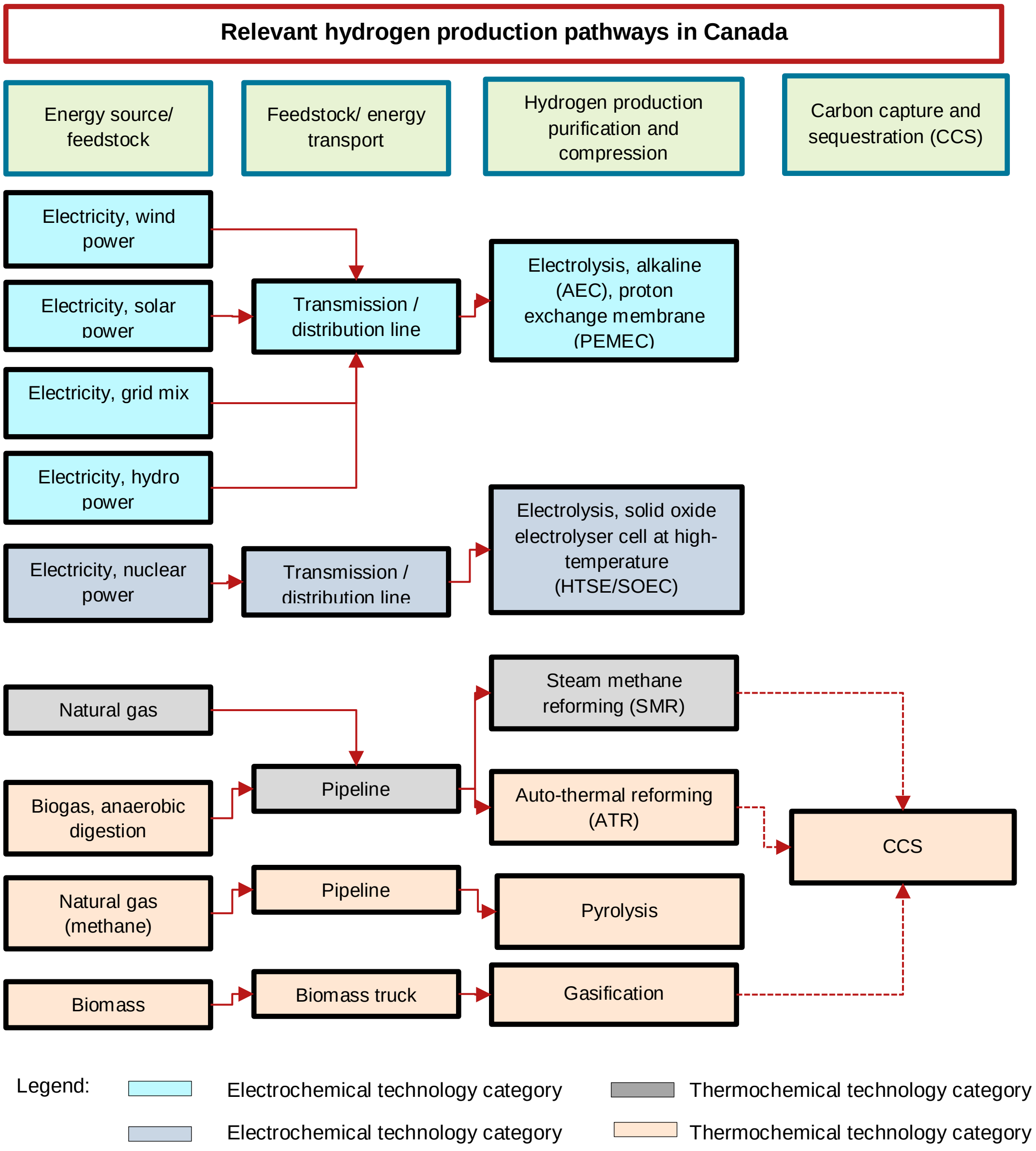


Figure 5-3: Overview of different hydrogen production pathways in Canada

LCA of hydrogen production pathways will be focused on two types of hydrogen technology categories, as follows:

i. Thermochemical, which will consider different configurations of feedstock and type of processes:
    a. Steam methane reforming (SMR) using natural gas with/without CCS and biogas via anaerobic digestion with/without CCS;
    b. Auto-thermal reforming (ATR) using natural gas with/without CCS and biogas via anaerobic digestion with/without CCS;
    c. Gasification using biomass with/without CCS
    d. Pyrolysis, using natural gas (methane);
ii. Electrochemical, which will consider several configurations of energy sources and type of electrolysers:

a. Electrolysis using different renewable electricity sources (electricity grid, hydroelectricity, wind, and solar).
b. Electrolysis using alkaline (AEC) and proton exchange membrane (PEMEC) electrolysers.
c. Electrolysis using nuclear electricity and solid oxide electrolyser cell at high-temperature (HTSE/SOEC)

The Hydrogen Strategy for Canada (NRCan, 2020) indicates that annual hydrogen production in Canada is 3 million tonnes via steam methane reforming of natural gas. Since SMR of natural gas without carbon capture is the best available technology to produce hydrogen in Canada, this is assumed to be the baseline pathway to estimate the threshold of the life cycle GHG emissions of hydrogen production pathways in Canada.

5.1.3.2.5 Comparisons between systems

The equivalence of the hydrogen product systems is a requirement to compare the carbon intensities between hydrogen product systems in this study (ISO, 2020). To determine this equivalence, the following life cycle assessment elements need to follow identical carbon footprints quantification criteria (ISO, 2018). For all the hydrogen production pathways to be evaluated in this study, referring ISO 1467:2018, the following criteria is applied for the goal and definition stage:

I. Product system definition and description are identical
II. Functional unit is identical
III. System boundary is equivalent
IV. Criteria for inclusion of inputs and outputs are equivalent
V. Assumptions are the same
VI. Specific GHG emissions and removal are treated identical
VII. Units are identical

The following criteria is applied for the life cycle inventory and LCIA stages:

I. Data collection methods are equivalent
II. Data quality requirements are the same
III. Calculation procedures are identical
IV. Allocation of the flows are equivalent
V. Applied GWPs are identical.

5.1.4 System boundaries definition

The system boundary identifies all the process to be included in the life cycle assessment (ISO, 2006b, 2018).

Overall the system boundary approach that comprises all the elements of the hydrogen value chain is called ‘well-to wheel” approach considering all the life cycle stages options from raw materials acquisition and transportation through hydrogen production up to transportation to end users and use of hydrogen. It is illustrated in Figure 5-4.

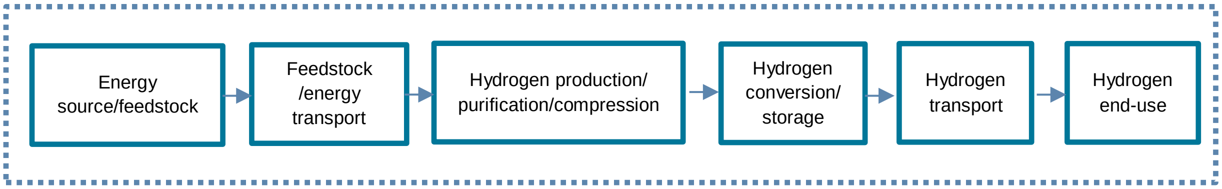


Figure 5-4: Overall system boundary of hydrogen value chain based on a “well-to-wheel” approach

The boundaries of the value-chain elements covered in the emissions accounting of certification schemes will have substantial implications for emission-reduction incentives and balance of international tradability (White et al., 2021). Table 4-2 outlines the current active or proposed hydrogen certification schemes in the world. The most common system boundary approach in various certification schemes is the point of production approach, which allows calculation of the GHG emissions of the hydrogen produced at the gate of the production plant, with compression and purification included (BEIS, 2021; CertifHy, 2019; IPHE, 2021; TÜV-SÜD, 2021).

Furthermore, harmonization of system boundaries of hydrogen production systems, as it is proposed in several publications according section 4.2.1 in this report, intends to improve comparison between LCAs for different hydrogen production systems. Based on that perspective, a harmonized system boundary for hydrogen production systems are illustrated in Figure 5-5. This hydrogen production LCA study adopted a “well-to-gate” system boundary approach that takes into account a foreground and background system. The foreground system comprises the following sub-systems and processes:

i. (SS1): Thermochemical hydrogen production system, includes feedstock extraction and production of natural gas or biomass and transportation using pipelines and trucks, respectively. For electrochemical hydrogen production system, include energy sources as renewable, non-renewable, and grid mix to produce electricity, which is delivered via transmission /distribution lines.
ii. (SS2): Hydrogen production and purification process related to thermochemical and electrochemical hydrogen energy systems. If it is applicable, carbon capture and storage process is included.
iii. (SS3): Hydrogen compression.

The background system provide carbon emissions factors of inputs such as energy (electricity/ heat) and materials to the foreground system.

This “well-to-gate” system boundary includes Scope 1, Scope 2, and partial upstream Scope 3 emissions associated to raw materials acquisition, hydrogen production, and transportation processes from the foreground and background systems. Scope 1, 2, and 3 are defined by the Greenhouse gas protocol: Product life cycle accounting and reporting standard by WRI (2004).

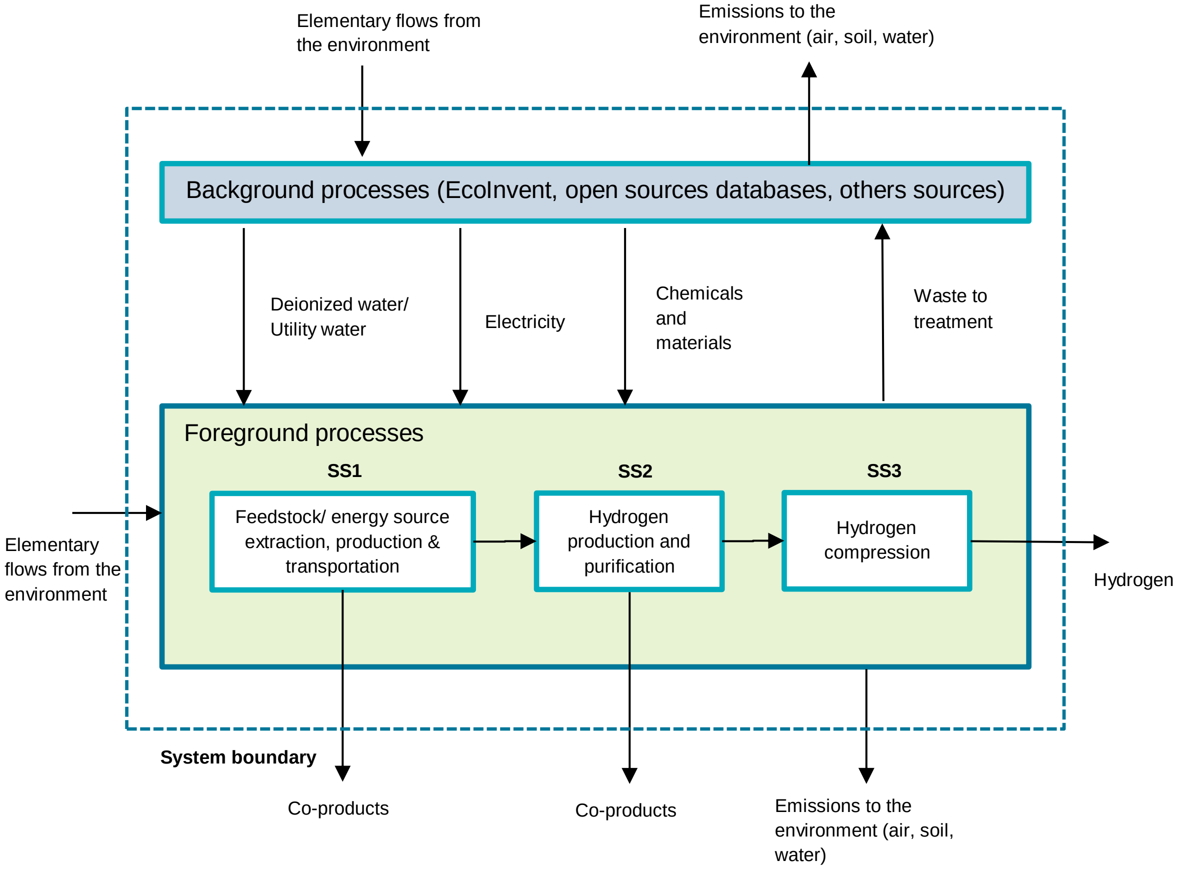


Figure 5-5: Well-to-gate system boundary for hydrogen production in Canada

5.1.4.1 Excluded processes

The life cycle inventory for each hydrogen production pathway only considers the materials and energy of the unit processes that are part of the "well-to-gate" system boundary with exception of unit processes that generate downstream scope 3 emissions (out of scope, "gate-to-grave" boundary) and the embedded emissions in capital goods (CAPEX). The latter are excluded considering the relative small impact of adding these emissions to emissions associated to both fossil and renewable sources-based pathways (Hydrogen-Council, 2021; IPHE, 2021; Pehl et al., 2017).

The emissions from the following activities are not included in the baseline requirements (CertifHy, 2019; ECCC, 2021; IPHE, 2021):

i. Construction, manufacturing, and decommissioning of the capital goods (including hydrogen production device, hydrogen production plant, associated plant components/auxiliary equipment, etc.),
ii. Business travel, employee commuting, and upstream leased assets,
iii. Transport and supply of the hydrogen to the consumers,
iv. Use of the hydrogen, and
v. Product end-of-life

These exclusions are applied consistently through all hydrogen production pathways.

5.1.4.2 Cut-off criteria

Overall all the elementary, product, and energy flows of the processes defined in the system boundary with a significant contribution to the GHG emissions are included. However, any material/energy flow with ineligible contribution should be excluded from the system boundary to be evaluated (ISO, 2006b). For this LCA study, the environmental significance criterion is used to decide which inputs are included in the LCA. If there is an input with cumulative GHG emissions contribution less than 5% of the total carbon intensity of the product system, it should be excluded. Regarding the outputs to be excluded, the GHG emissions related to elementary flows with a contribution less than 1 % will be excluded.

5.1.5 Development and implementation of a life cycle inventory of hydrogen production pathways

The life cycle inventory (LCI) is a collection of input/output data in accordance with ISO 14040/44:2006 standards that can be used to carry out life cycle impact assessment. LCIs can be developed using primary or secondary data sources. In strict sense, primary data are based on measurements or derived from measurements of actual plants and production sites. However, in practice, many other data sources can be used to generate primary data such as patents, process engineering models, stoichiometric models, product or feedstock specifications and legal limits (ILCD, 2010b).

On the other hand, secondary data refers to data that are not based on measurements or derived from measurements of foreground system under study. Secondary data also represents the inventory datasets obtained from third parties, average or aggregated data from databases and national inventories, which are typically used to model the background system. Foreground system can contain secondary data as well. For example, literature data used to address data gaps in foreground system are still considered secondary data (ILCD, 2010b).

NOTE: In the two hydrogen pathways presented in this report, the data generated specifically from process modelling and simulation results are characterized as primary data. Foreground system is typically modeled using primary data. It is important to note that the simulation outputs in this study were obtained from I-BIOREF software, which calculates mass balance of input and output materials. Since I-BIOREF does not include all the existing configurations of the unit processes used for the two hydrogen pathways, some of the unit processes such as SMR reactor, pressure swing adsorption (PSA) off-gas combustion topped up by natural gas to provide the SMR reactor heat duty, and the hydrogen cooling unit for both SMR and alkaline electrolysis processes were previously simulated in ASPEN software. However, energy balance and optimization was not performed using I-BIOREF for the two hydrogen production processes and will be updated in the subsequent reports of LCA of hydrogen production pathways.

In addition, LCI data can be presented either as unit process or aggregated process data sets. Unit process datasets are created by quantifying inputs and outputs in regards to a reference flow. The inputs and outputs are typically obtained by a simulation or mathematical modeling. On the other hand, the aggregated datasets are obtained by combining multiple unit process datasets or aggregated datasets. Aggregated datasets are useful in reducing the complexity of a system containing multiple unit process datasets or in using data without disclosing confidential/proprietary information. In this project, both unit process and aggregated process datasets are used (Sonnemann, 2011).

Based on ISO 14040/44:2006 standards, the generation of unit process dataset is a 5 step process (Sonnemann, 2011).

i. Preparation of inventory list of inputs and outputs
ii. Define mathematical/modeling relationships
iii. Collection of raw data required
iv. Performing the necessary calculations

v. Provision of supportive information

For the two hydrogen pathways presented in this report, the process modelling and simulation covers the steps 2 to 4, which will be described in section 6. Although, 5 step process is typically sufficient in generating inventories, further considerations are needed in order to compare inventories available in the literature, data quality assessment, filling data gaps and selection of background system datasets. Hence, the methodology shown in Figure 5-6 is developed in this project for development of life cycle inventories.

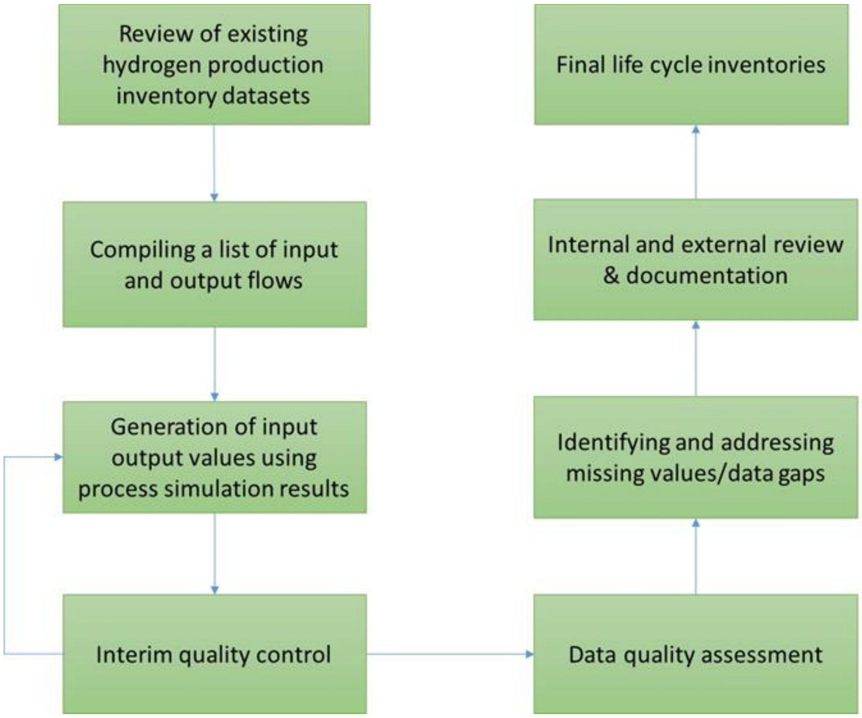


Figure 5-6: Steps taken in developing life cycle inventory datasets for hydrogen production pathways

5.1.5.1 Review of existing hydrogen production inventory datasets in literature

A review is performed for selected hydrogen production pathways in section 5.1.3.2.4 with similar system boundaries defined in the current study. The following data was collected during the literature review of inventory datasets.

i. Input flows and values
ii. Output flows and values
iii. Functional unit
iv. Background system database references
v. Data quality

5.1.5.2 Compiling a list of input and outputs flows

The first step in creating a life cycle inventory is to create a list of potential inputs and outputs related to the unit process under study. Since the current study is using a system representation based on simulation models, a list of input and outputs is developed during the literature review. The names of the inputs and outputs, the type differentiating whether it is a flow to or from technosphere (background system) or elementary flow from or to environment and any background database process connectives should be listed.

5.1.5.3 Life cycle inventory based on process simulation data and interim quality control

Conversion of raw or modeling data to unit process data involves following steps (ILCD, 2010b).

1. Correct scaling of inputs and outputs to the functional unit/reference flow. In the current study, this unit is 1 kg of H_2 production.
2. Documentation of all data treatment steps involved such as unit conversions and assumptions.

Once preliminary data has been generated using simulation models or other data collection methods, it is recommended to check the quality of data before finalization of inventories and provide the feedback to process simulation for any required changes (ILCD, 2010b). This interim quality control typically includes evaluation in terms of identifying significant issues, completeness check, sensitivity check and consistency check.

5.1.5.4 Data quality assessment

5.1.5.4.1 Data quality indications

The use of data quality indicators (DQI) is standard practice in evaluating the data quality of LCIs. The most commonly used data quality assessment system is the pedigree matrix that evaluates the data in terms of multiple criteria (Edelen, 2016; Wernet, 2016). Data quality assessment provides a measure of representativeness of the unit process being studied and results are typically included as metadata along with LCI. In some cases, data quality assessment is used to achieve certain required data quality goals required by the analysis. Following DQIs are typically used in measuring data quality of each flow in a unit process data set.

- i. Reliability
- ii. Completeness
- iii. Time related appropriateness
- iv. Geographical appropriateness
- v. Technological appropriateness

Each DQI is given a score of 1 to 5 upon evaluation of data quality (Table 5-2). Reliability provides indication of quality of data collection and validation methods. Completeness evaluates the robustness of sampling methods and amount of data points collected. Time related and geographical appropriateness measures the representativeness in terms of correct geography such as country or region and the age of the data. Technological appropriateness measures the gap between goal and scope of LCA study and actually represented technology.

Table 5-2: Data quality indicator and their scoring guidance for flows (Wernet, 2016)

Indicator/score	1	2	3	4	5 (default)
Reliability	Verified data based on measurements	Verified data partly based on assumptions or non-verified data based on measurement	Non-verified data partly based on qualified estimates	Qualified estimate (e.g. by industrial expert)	Non-qualified estimate
Completeness/data collection methods	Representative data from all sites relevant for the market considered, over an adequate period to even out normal fluctuations	Representative data from >50% of the sites relevant for the market considered, over an adequate period to even out normal fluctuations	Representative data from only some sites (<<50%) relevant for the market considered or >50% of sites but from shorter periods	Representative data from only one site relevant for the market considered or some sites but from shorter periods	Representativeness unknown or data from a small number of sites and from shorter periods

Time related appropriateness	Less than 3 years of difference to the time period of the dataset	Less than 6 years of difference to the time period of the dataset	Less than 10 years of difference to the time period of the dataset	Less than 15 years of difference to the time period of the dataset	Age of data unknown or more than 15 years of difference to the time period of the dataset
Geographical appropriateness	Data from area under study	Average data from larger area in which the area under study is included	Data from area with similar production condition	Data from area with slightly similar production conditions	Data from unknown or distinctly different area
Technological appropriateness	Data from enterprises, processes and materials under study	Data from processes and materials under study (i.e. identical technology) but from different enterprises	Data from processes and materials under study but from different technology	Data on related processes or materials	Data on related processes on laboratory scale or from different technology

The data quality assessment can also be incorporated in the uncertainty analysis during life cycle impact assessment. Necessary formulas and probability distributions can be found in the literature (Wernet, 2016). In addition to flow related DQI, further DQIs related to process data quality has been developed as shown in Table 5-3.

Table 5-3: Data quality indicator and their scoring guidance for processes (Edelen, 2016)

Indicator/score	1	2	3	4	5 (default)
Process completeness	>80% of determined flows have been evaluated and given a value	60-79% of determined flows have been evaluated and given a value	40-59% of determined flows have been evaluated and given a value	<40% of determined flows have been evaluated and given a value	Process completeness not scored
Process review	Documented reviews by a minimum of two types of third party reviewers	Documented reviews by a minimum of two types of reviewers, with one being a third party	Documented review by a third party reviewer	Documented review by an internal reviewer	No documented review

5.1.5.5 Addressing data gaps and final life cycle inventories

As discussed in section 5.1.5.3, some flows are missing in the initial LCIs developed. There are multiple ways of handling missing data including calculations, averages from literature and expert estimates. In this study, we followed the guidance provided by ILCD (ILCD, 2010b), which has been illustrated in Figure 5-7. First and second steps in the procedure are the identification of the missing data and assess their relevance in overall project scope.

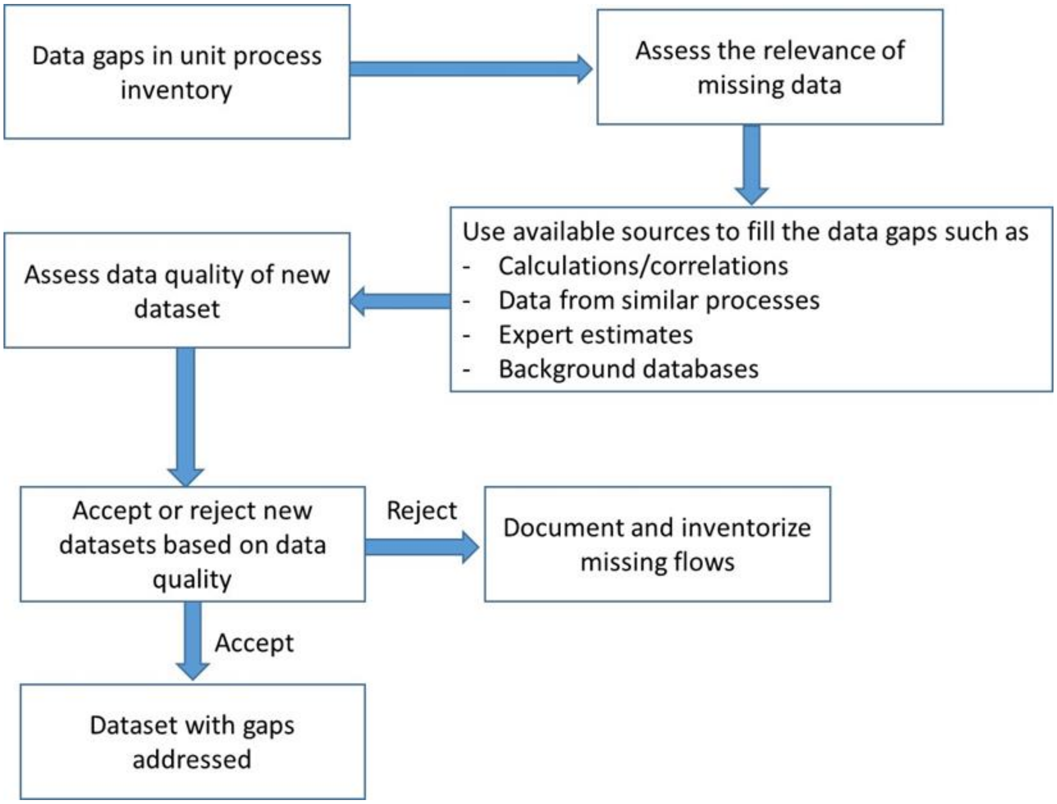


Figure 5-7: Procedure for addressing data gaps and missing data in life cycle inventories.

Then final life cycle inventories are developed and take into account the two types of datasets: the foreground and background inventory datasets.

5.1.5.6 Life cycle inventory modelling approach

The two main LCI modelling principles are the attributional and consequential modelling as two alternatives to model the product system.

While attributional LCA aims to quantify the environmental impacts of a product system along with its life cycle using average data, the consequential LCA intends to evaluate the changes on environmental impacts as a result of the production, use or disposal of a product using marginal data.

In the case of the LCA hydrogen production, the attributional modelling is adopted since the goal of this LCA is to quantify the GHG emissions for different hydrogen production pathways, instead of understand the impacts on other process or systems due to changes in hydrogen production.

5.1.5.7 Implementation of a publicly available Canadian LCI database of hydrogen production pathways

Life cycle assessment studies are increasingly detailed in order to more accurately model the products subject to the analysis. To do so, an LCA model of a product requires the integration of large number of other models of the components used in the product studied. In order to successfully carry out such integration, database of models need to be easily accessible in order for researchers to share models and integrate other’s models in their LCA model.

5.1.5.7.1 Harmonization of datasets

The harmonization of hydrogen production datasets were not carried out as a single set of processes were generated in the current project. However, initial guidelines were proposed to harmonize and integrate hydrogen production datasets from multiple sources.

i. Refine and complete the data quality indicators that describe fitness for purpose for datasets and studies for hydrogen and hydrogen supply chain.
ii. Apply the indicators for datasets and studies.
iii. Develop a concept for displaying the indicator results.
iv. Develop a minimum scoring for the indicators.
v. Develop an approach for aggregating data quality results over a life cycle.

5.1.5.7.2 Implementation of an openLCA collaboration server

Lifecycle analysis studies are increasingly detailed in order to more accurately model the products subject to the analysis. To do so, a lifecycle analysis model of a product requires the integration of large number of other models the components used in the product studied. In order to successfully carry out such integration, database of models need to be easily accessible in order for researchers to share models and integrate other's models in their life cycle analysis model.

In this aim, NRC undertook the creation of a publicly accessible web server using the web application openLCA collaboration server developed by GreenDelta since 2006.

5.1.6 Life cycle carbon intensities calculations for hydrogen production

The accounting of life cycle GHG emissions intensity is carried out in accordance with the GHG Protocol (WRI, 2004) and ISO 14067:2018 (ISO, 2018). Assumptions and allocation procedures should be documented as well.

The following requirements to calculate carbon intensities for hydrogen produced in the determined system boundary are as follows:

5.1.6.1.1 Emissions accounting

Emissions consider all Scope1 and 2, and partial Scope 3 emissions occurring in the "well-to-gate" system boundary. Co-products emissions can be calculated based on allocation procedures defined in section 5.1.6.1.3. Carbon capture and storage (CCS) emission removals are defined according IPCC guidelines.

The net GHG emissions accounted for each hydrogen production pathways is the total emissions subtracted by CCS removal and co-products accounted emissions (Figure 5-8).

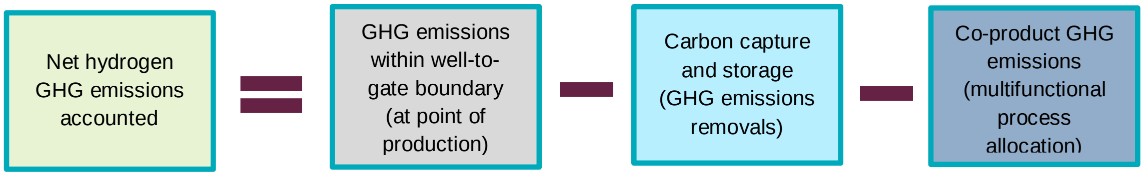


Figure 5-8: Carbon emissions accounting for hydrogen production

Total GHG emissions accounted for most of hydrogen production pathways consider: (i) combustion emissions, e.g. flue gases from natural gas combustion; (ii) energy supply emissions, including electricity and natural gas; (iii) embodied emissions, which include upstream emissions associated with any input stream to the product system, e.g. natural gas is used as feedstock in the steam methane reforming pathway, where the embodied emissions comprise emissions from natural gas extraction, production, transportation, and fugitive emissions from leakages or losses.

5.1.6.1.2 Mass balance.

To ensure physical traceability for materials at all stages of hydrogen production value chain. Currently this requirement is in TÜV-SÜD (2021) and under development in CertifHy (BEIS, 2021).

5.1.6.1.3 Co-product allocation

Production of hydrogen under different pathways results in a range of waste materials for further treatment, by-products, and co-products. In the case of co-products, the total emissions from hydrogen production is distributed or allocated between the hydrogen product system and co-products, which are subject to valorization as an input into another product system.

For waste products and CO_{2e} emissions there are no allocation. These by-products are assumed to be co-products.

Allocation procedures for solving multifunctionality with co-products are indicated in ISO 14044:2006, which considers allocation should be avoided by dividing the unit process to be allocated into two or more sub-processes and collecting the input and output data related to these sub-processes or using system expansion. If allocation cannot be avoided, physical partitioning can be applied. However, in ISO 14044:2006/AMD 2:2020, Annex D document, no prioritization is recommended between system expansion and physical allocation. Following ISO 14067:2018, the LCI is based on materials balances between input and output and allocation procedures should be consistently applied to inputs and outputs of the product system under study. The current allocation methods could be applied in the following order:

i. Partitioning, physical: mass, energy content.

If allocation cannot be avoided, the inputs and outputs of the system should be partitioned between its different products or functions in a way that reflects the underlying physical relationships between them (ISO, 2006b). Physical partitioning is applied if there is a physical relationship between inputs/outputs/co-products on a mass basis or energy content basis. The latter is the most appropriate to hydrogen production due to its high energy to mass ratio, however not all co-products, especially non-energy co-products, contain useful energy such as oxygen from the electrolysis pathways, where another method could be used (IPHE, 2021). Energy content for hydrogen is the lower heating value (LHV) equals to 119.9 MJ/kg.

This allocation method is recommended to be applied when the production of co-products in a multifunctional process can be independently changed and as a consequence there are variations on amounts of inputs required, emissions released, and waste generated.

ii. System expansion.

ISO 14044:2006 indicates that allocation can be avoided by expanding the product system to include additional functions related to the co-products. System expansion considers co-products have alternative products to substitute its environmental burdens in the product system under study. The GHG emissions from the substituted product are withdrew from the total emissions of the product system. Figure 5-9 illustrates an example of system expansion procedure.

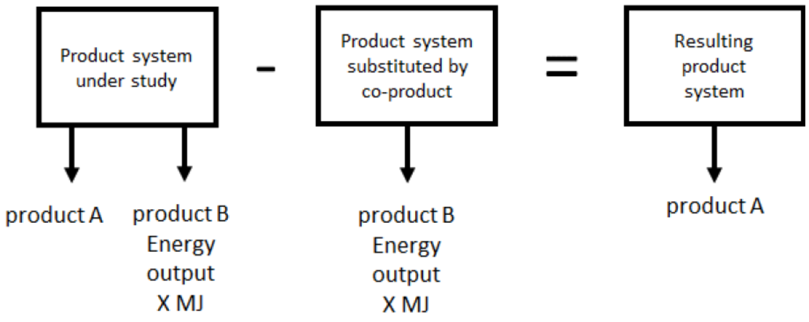


Figure 5-9: System expansion procedure according ISO: 14044:2006/AMD 2:2020

Although system expansion could be a direct alternative to avoid allocation, there is a potential issue if there are different substitute pathways for co-products because it could lead to a high variability of results. It is important to identify and defined a unique substitute system of a specific co-product to be used in a hydrogen certification scheme.

For instance in the case of co-products from the hydrogen product system by SMR pathway, system expansion could be applied for excess electricity or steam generated at hydrogen production facility. These electricity and steam co-products can be used for other process in another product system.

iii. Economic value

Economic allocation is usually based on the revenue obtained from co-products. However market prices are subject to a high variability and uncertainty. Therefore, this type of allocation can be used when physical allocation or system expansion cannot be applied.

In this hydrogen LCA study, allocation for each type of pathway will be evaluated on a case-by-case basis.

5.1.6.1.4 Treatment of electricity

In order to maintain consistency for the quantification of GHG emissions intensity along the hydrogen production pathways, ISO:14067:2018 indicates GHG emissions associated with the use of electricity come from (i) life cycle GHG emissions from the electricity supply system without emissions embedded associated to capital goods and (ii) electricity generation as well transmission and distribution losses.

Other considerations to take into account (ISO, 2018) are as follows:

5.1.6.1.4.1 On-site generated electricity

On-site generated electricity is part of Scope 1. Hydrogen production through electrolysis uses electricity as energy source. This electricity can be off-grid electricity generated from renewable sources such as wind, solar, and hydro. In this case, GHG emissions from this electricity source are assumed as zero.

5.1.6.1.4.2 Electricity from the grid

Electricity from the grid is part of Scope 2. Average grid GHG emissions factors associated to a specific electricity grid in a province can be obtained from trusted LCI databases if there is no available information from the electricity supplier. Emissions from electricity consumed by the hydrogen production facility comprise upstream emissions, electricity production, and downstream emissions with all the electricity generation, transmissions, and distribution losses. Emissions are calculated as the amount of electricity consumed multiplied by the average grid emission factor expressed in kilograms of CO_{2e} per kilowatt-hour.

5.1.7 Life cycle impact assessment

Perform the life cycle impact assessment (LCIA) by classifying the inventory substances in inputs and outputs according to the environmental selected impact categories. Based on the classification, the environmental impacts are characterized by means of a set of characterization factors that are specific to the substance, the impact and the selected assessment method (e.g., ReCiPe, CLM, IPCC, and VDI, etc.).

5.1.7.1 Selection of an impact assessment method

LCIA methods are applied to quantify environmental impacts based on LCI data.

As per the goal and scope definition for this hydrogen LCA, the environmental impact category selected is climate change. Following ISO 14067:2018, the potential climate change impact of each GHG emitted and removed by the product system is calculated by multiplying the mass of GHG released or removed by the 100-year global warming potential (GWP) given by the Intergovernmental Panel On Climate Change (IPCC) in units of kg CO_{2e} per kg emission. According the IPCC's Fifth Assessment Report (AR5) (Myhre & T. Nakajima, 2013) the characterization factors for a period of 100 years (GWP100) that are taking into account in this study for calculating carbon intensities are listed in Table 5-4.

To be consistent with the approach of Environment and Climate Change Canada (ECC)'s Fuel LCA model (ECCC, 2021) and other carbon intensities initiatives in Canada as the Canadian National Inventory (ECCC-NIR, 2021), the biogenic carbon dioxide are assumed to be zero and the CO_2 emissions or uptake from direct land use change have the same impact factor as fossils CO_2.

Table 5-4: Global warming potential (GWP100) of selected greenhouse gases

GHGs	AR5 CO2e (kg/kg)
Carbon dioxide (CO_2)	1
Carbon dioxide, biogenic (CO_2)	0
Carbon dioxide, land use change (CO2)	1
Methane, fossil (CH_4)	30.5
Methane, biogenic (CH_4)	27.75
Nitrous oxide (N_20)	265

The LCIA's results are expressed in $kgCO_{2e}$/ kg H_2.

5.1.8 Limitations of hydrogen LCA methodology

As in ISO14067:2018, although the carbon intensity is an important and relevant environmental impact of hydrogen production along its life cycle, there are other environmental impacts related to areas of concern such as cumulative energy demand, resource depletion, among others, which might be relevant for a complete assessment of the environmental impact of hydrogen production. Decision making to minimize GHG emissions in a process may increase the effect from other environmental aspects. Future work should analyze the trade-off between impact categories.

The life cycle inventory datasets such as electricity or natural gas production only correspond to current Canadian values and are not taking into account prospective values as a result on changes on environmental or energy policies in Canada or technological improvements.

The hydrogen production life cycle inventory datasets are based on the results of a process modeling and simulation procedure to mitigate the lack of primary data from current hydrogen production processes in Canada. However, the model will be updated as primary data becomes available.

5.1.9 Results and discussion

Analysis and interpretation of the quantification of GHG emissions intensity, flow contribution analysis, and classification of hydrogen to be certified.

6 Steam Methane Reforming with Natural Gas: Baseline Pathway

The steam methane reforming (SMR) process is well-known and most mature hydrogen production pathway. In this section, SMR pathway with assumed system boundary, input assumptions and mass balance of the system is presented.

6.1 System boundary

The scope of the life cycle assessment of hydrogen production under the SMR pathway using natural gas is defined by identifying which processes are included and excluded in this LCA study. A general description of the SMR pathway system boundary is presented in this section.

Overall, a harmonized SMR system boundary is illustrated in Figure 6-1, showing which inputs and outputs flows should be included in this generalized SMR system boundary following the criteria indicated in section 5.1.4. Based on Figure 5-5, the foreground system comprises three subsystems, SS1 that considers the extraction and production of the feedstock, i.e. natural gas and its transportation through pipelines to the SMR plant; SS2 includes the feedstock pre-treatment (sulfur removal), and the hydrogen production and purification; and SS3 that refers to hydrogen compression to obtain hydrogen product that comply with the minimum specifications indicated in Table 5-1.

Briefly, the natural gas feedstock goes through a chemical desulfurization process using solvents and catalysts to further reduce the sulfur content in the gas. The separated sour gases from the desulfurization unit are sent to a LO-CAT® unit where hydrogen sulfide is oxidized by air and transformed into sulfur cake (waste product).

The clean gas – generally referred to as sweet gas – is rich in methane and therefore reformed in the reformer using steam as reforming agent and in the presence of a cobalt catalyst. Steam reforming as an endothermic reaction requires heating energy, which is provided by combusting process off-gases including those from the LO-CAT® unit and the downstream Pressure Swing Adsorption (PSA) unit, as well as natural gas as fuel. Methane as well as other alkanes are transformed into syngas components via the reforming process and exit the reactor at a high temperature (above 900 C) which passes through a heat recovery unit system to exchange their heat, relatively cool down and produce steam. Excess steam could be a co-product used to provide heat or produce electricity that could be sold to the electricity grid system.

The product gas passes through a Water-Gas-Shift (WGS) reaction step, which uses steam to increase the hydrogen content and reduce carbon monoxide in the product gas mix. The WGS hydrogen-adjusted product goes through an adsorption process within the PSA unit, where hydrogen gas is separated. Finally, hydrogen gas is compressed using medium pressure compressors to 200 bar followed by cooling to reach the storage conditions. The emissions from this SMR process are off-gases from the reforming unit, primarily carbon dioxide (CO_2) that are completely emitted to the air. Carbon capture and sequestration unit (CCS) process is excluded from this pathway system boundary.

The following section will use this system boundary as blueprint to model and simulate a SMR process to produce hydrogen in the province of Alberta. More specification and assumptions will be also provided with a specific and detailed process diagram.

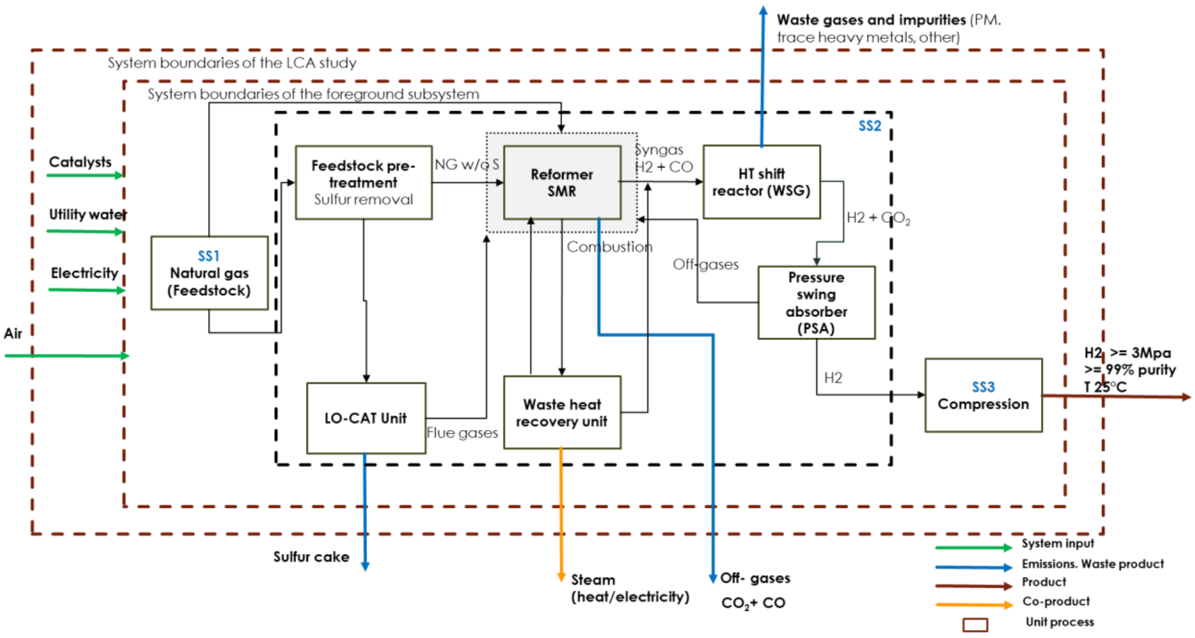


Figure 6-1: Well-to-gate system boundary for SMR hydrogen production using natural gas

6.2 Process modelling and simulation

6.2.1 Process description

Life cycle assessment requires chemical process analysis and establishing mass and energy balance. A process simulation of the SMR plant is, therefore, performed using I-BIOREF decision-support tool to provide mass balance (Benali, 2018; NRCan, 2021) Appendix 9.2, considering the unit operations included in the system boundary section. A general block flow diagram of the SMR pathway is illustrated in Figure 6-2, which simplified the basic structure of the simulated SMR system under study.

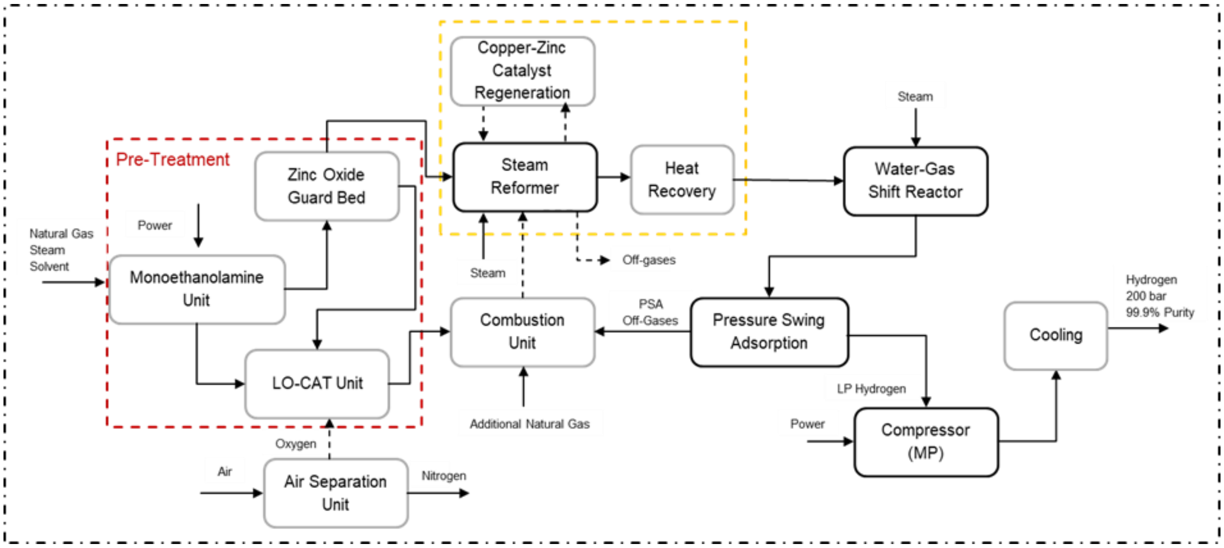


Figure 6-2: Block flow diagram of the SMR pathway

A detailed process diagram is shown in Figure 6-3 and the role and performance of each unit process is briefly described in this section.

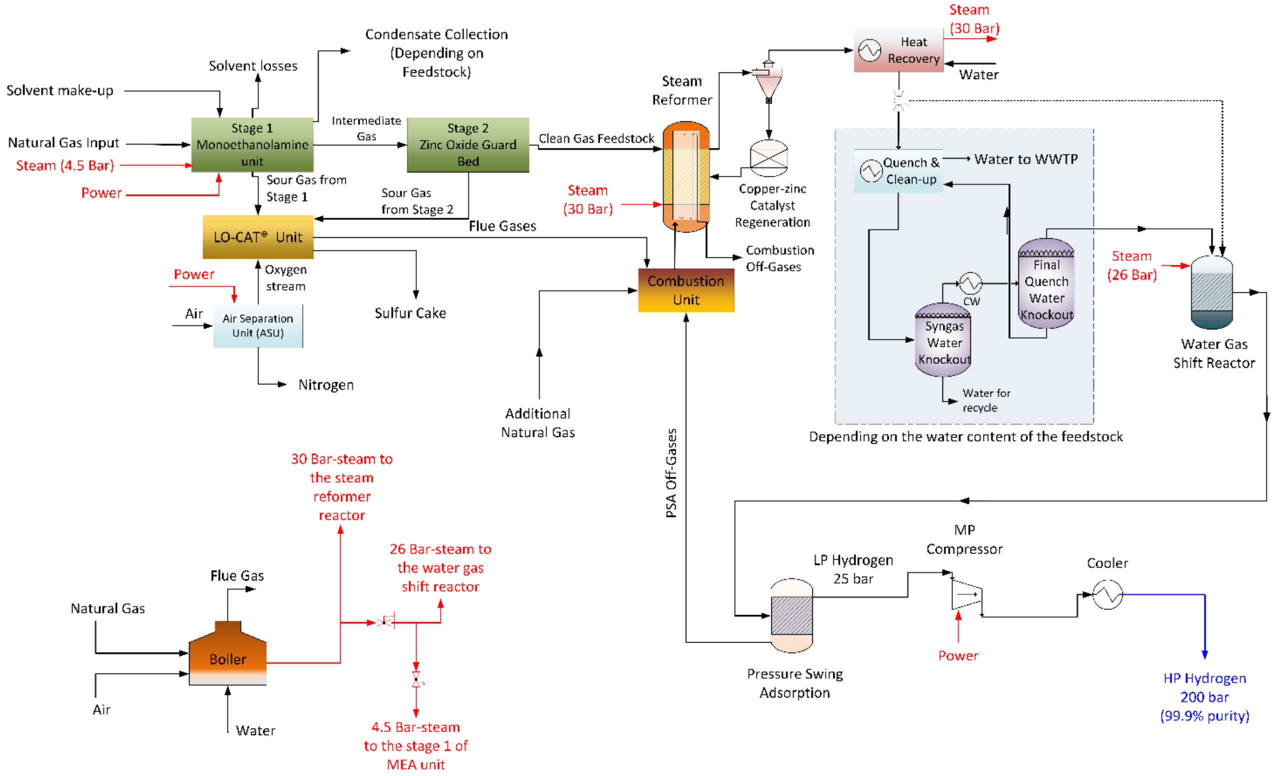


Figure 6-3: Process diagram of the steam methane reforming plant

6.2.1.1 Raw Gas Pre-treatment Unit

The considered SMR pathway of this study starts with the pre-treatment unit that includes desulfurization, zinc oxide guard bed, and LO-CAT® unit processes. The raw gas enters the desulfurization unit, which uses the monoethanolamine (MEA) solvent for absorbing H_2S and CO_2 from the raw gas. MEA offers high absorption rate and is readily available at low cost. It uses a 20% concentrated MEA which absorbs 0.4 mole acid gas per mole of MEA (Swanson, Platon, Satrio, Brown, & Hsu, 2010). The removal rates for H_2S and CO_2 are 99% and 90%, respectively (Swanson et al., 2010).

The partially stripped raw gas from H_2S and CO_2 is then entered in a zinc-oxide guard bed unit for further reduction of sulfur. Zinc oxide is the most widely used adsorbent for hydrogen sulfide removal from natural gas and has good chemical stability and allows for a quick reaction at high temperatures (Swanson et al., 2010; Yang, Sothen, Cahela, & Tatarchuk, 2008). The polishing step is necessary to bring the sulfur content down to ppb level (Swanson et al., 2010) required for high purity hydrogen production. Eq (1) summarizes the reaction that takes place in this unit:

$$ZnO + H_2S \rightarrow ZnS + H_2O \qquad (1)$$

Stripped sulfur from MEA and Zinc oxide units in the form of H_2S is then directed to the LO-CAT® unit for oxidation by air. LO-CAT® is a patented process with a demonstrated hydrogen sulphide (H_2S) removal efficiencies in excess of 99.9% and recovering elemental sulphur from hydrogen sulphide (McManus & Kin, 1986). The H_2S is absorbed, ionized and oxidized from H_2S to S. Thereafter, it reduces iron, absorbs O_2 and oxidizes iron. The conversion of H_2S to S is performed using chelated-based iron catalyst. The LO-CAT® includes a venturi precontactor, absorber, air blower, air-blown oxidizer, solution circulation pump, and solution cooler. The unit converts H_2S to a sulfur cake as in Eq (2) and removes > 99.9% of the incoming H_2S. Major advantages of LO-CAT® process, based on reduction-oxidation chemistry, are its low catalyst regeneration requirements and benign environmental impacts of catalyst. Two reduction-oxidation reactions take place: one in the absorber zone where H_2S is converted to S, and one in the oxidizer zone where the catalyst is regenerated.

$$H_2S + \frac{1}{2} O_2 \rightarrow H_2O + S \qquad (2)$$

The sulfur cake can either be stockpiled and sent to landfill or sold as product. Due to the presence of methane in outlet gas of the LO-CAT® unit, the off-gases are directed to the combustion unit to off-set part of the required natural gas for heat generation.

6.2.1.2 Air Separation Unit

Oxygen demand of the LO-CAT® unit is provided from an air separation unit. This unit is designed to produce high purity oxygen for the feedstock pre-treatment unit in large volumes. A two-column cryogenic oxygen and nitrogen separation is used followed by oxygen compression and nitrogen purge (Swanson et al., 2010). The air is pre-cooled via exchanging heat with exiting nitrogen. It is assumed that the produced oxygen has 99.3% purity.

6.2.1.3 Steam Methane Reforming Unit

Pretreated natural gas - after the zinc oxide unit – is then introduced into the steam reformer unit. SMR is a mature technology, the most common and well-known process for its low-cost hydrogen production and a key technology for near-term hydrogen production (DOE, 2022) which accounts for around 80% of hydrogen production in the US and 40% in the world (Muradov, 2015). Syngas consisting of hydrogen, CO_2, and a relatively small amount of CO is the product of this catalytic-endothermic reaction between the steam and methane. Steam reforming process is an endothermic process, and the heat must be supplied for the reaction to proceed. According to Figure 6-3, the combustion unit provides the required heat for this reaction. The catalyst regeneration unit is also coupled with SMR for the regeneration of the used catalyst. In this study, a stoichiometric reaction with a methane conversion of 80% is assumed.

6.2.1.4 Water Gas Shift Unit

Maximizing the hydrogen and minimizing the carbon monoxide at the same time is the main objective of the Water Gas-Shift unit. The produced syngas from SMR unit is the feed for the WGS reactor and as it is shown in Eq (3), carbon monoxide reacts with water to adjust the H_2: CO ratio of the output stream at an assumed value of 2:1.

$$CO + H_2O \Leftrightarrow CO_2 + H_2 \qquad (3)$$

According to the application, the WGS could be designed as a two-stage reactor (high and low temperature). In this study, WGS process is modeled as a single reactor at low temperature and medium pressure. Detailed operating conditions of the reaction is provided in Table 6-2.

6.2.1.5 Pressure Swing Adsorber Unit

To separate the hydrogen from the mixed gas stream exiting the WGS unit, a pressure swing adsorption (PSA) unit is designed to deliver the hydrogen with 99.9% purification. The light gases such as CO, CO_2, and CH_4 are adsorbed in this unit with two trains and six reactors. PSA adsorbers are filled with a 2:1 activated carbon/molecular sieves packing or activated carbons only. In this study, we have considered only activated carbons as adsorbers. As in the case of LO-CAT® off-gases, PSA off-gases are also combusted to provide a portion of the heat that the SMR reactor requires.

6.2.1.6 Hydrogen Compression Unit

For this study, the final pressure of the hydrogen is assumed to be 200 bar for the storage purposes and thus a compression step is required. A medium pressure compression train with three stages is modeled in this regard and based on assumed pressure of the outlet H_2; a heat exchanger is also considered for cooling the compressed hydrogen down to the storage temperature of 25°C. An isentropic efficiency of 81% has been considered for this study, which is the average value (72% and 90%) of a compressor isentropic efficiency based on different references (Campbell, 2014, 2015).

6.2.2 Input assumptions

The main input assumptions of the pathway are as follow:

I. Natural gas of Alberta with the density of 0.717 m^3/kg was considered for both feedstock and fuel (energy source for combustion and steam generation). The composition of natural gas is assumed to be that of Enbridge and is provided in Table 6-1.
II. Electricity mix source is from Alberta and its consumption is estimated based on the process electricity demand.
III. High quality deionized water is used for steam generation.
IV. The off-gases from the LO-CAT® and PSA processes in this study are combusted for two reasons: burning methane existing in the stream and providing heat required for the SMR unit leading to saving utility natural gas.
V. A stoichiometric reaction was considered for modeling the SMR reaction with a methane conversion of 80% and using cobalt as catalyst.
VI. An equilibrium reaction was used for modeling of water gas shift reaction and a downstream H_2:CO molar ratio of 2:1 was considered.
VII. For the WGS reaction, Cu-Zn-Al catalyst is used with a mass composition of: CuO: 40%, Zn: 45%, and Al_2O_3: 15%. The catalysts are replenished every 3 years.
VIII. For the pre-treatment of raw natural gas, monoethanolamine is used as the chemical desulfurization process.
IX. PSA bed is filled with activated carbon molecular sieves. The hydrogen separation efficiency from the gas mix is 85%.
X. No mass loss is considered in the compression stage.
XI. Oxygen purity from the ASU is 99.3 wt%.
XII. Hydrogen purity from the PSA unit is 99.9 wt%.
XIII. Sulfur removal efficiency of LO-CAT® unit is 99.9%.

Table 6-1: Natural gas weight composition (Enbridge, 2021)

Component	% Mass
Nitrogen	0.8%
Carbon Dioxide	0.8%
Methane	90%
Ethane	7.6%
Propane	0.5%
Butane	0.1%
Pentane	0.1%
Hexane	0.04%
Hydrogen Sulfide	0.04%
Oxygen	0.02%

6.2.3 Mass balance

Table 6-2 shows the inputs and outputs of the SMR pathway alongside the required energy. The calculated values are based on mass balances, as well as thermodynamics and kinetics that are all embedded in NRCan's I-BIOREF software.

Table 6-2: Mass balance of the SMR pathway

	Item	Unit	Amount	Reference
Pre-Treatment Unit (MEA + Zinc Oxide guard bed)	Input Natural Gas to MEA	tonne/day	517.3	Calculated based on mass balance
	Input Steam to MEA	tonne/day	7.33	Calculated based on mass balance
	Pressure of input steam to MEA	bar	4.5	A. Dutta and Phillips (2009)
	Required MEA solvent	tonne	543	Based on assumptions in the study by A. Dutta and Phillips (2009)
	Required make-up MEA solvent	tonne/day	0.05	Based on assumptions in the study by A. Dutta and Phillips (2009)
	Temperature of MEA absorber unit	°C	60	A. Dutta and Phillips (2009)
	Pressure of MEA absorber unit	kPa	241	A. Dutta and Phillips (2009)
	Temperature of zinc oxide unit	°C	340	A. Dutta and Phillips (2009)
	Pressure of zinc oxide unit	kPa	100	A. Dutta and Phillips (2009)
	Power consumption MEA	MWh/day	40.12	Based on assumptions in the study by A. Dutta and Phillips (2009)
	Zinc Oxide	tonne	36*	Based on assumptions in the study by A. Dutta and Phillips (2009)
Air Separation Unit	Input oxygen	tonne/day	0.09	Calculated based on mass balance
	Input nitrogen	tonne/day	0.29	Calculated based on mass balance
	Power consumption	MWh/day	0.03	Based on assumptions in the study by A. Dutta and Phillips (2009)
	Temperature	°C	-173.15	Schenk, Sakizlis, Perkins, and Pistikopoulos (2002)
LO-CAT® Unit	Temperature	°C	25	Merichem (2022)
	Pressure	kPa	100	Hydrocarbon (2022)
	Input sour gas	tonne/day	23.5	Calculated based on mass balance
	Output sulfur	tonne/day	0.18	Calculated based on mass balance
	Output water	tonne/day	0.10	Calculated based on mass balance
Boiler (steam generation for the process)	Steam generated (required for the process)	tonne/day	66.29	Calculated based on mass balance
	Natural gas required for steam generation	tonne/day	9.19	Calculated using Aspen plus simulation
Combustion Unit (Heat generation for SMR)	Temperature	°C	900	Based on assumptions in the study by A. Dutta and Phillips (2009)
	Pressure	kPa	100	Based on assumptions in the study by A. Dutta and Phillips (2009)
	Supplemented natural gas	tonne/day	50.01	Calculated using Aspen plus simulation
	Off-gas from LO-CAT® (contains 75% methane)	tonne/day	23.58	Calculated using Aspen plus simulation
Steam Methane Reforming Unit	Input Natural gas (output of pre-treatment)	tonne/day	494	Calculated based on mass balance
	Input Steam	tonne/day	403.27	Calculated based on mass balance

	Required catalyst	tonne	3.29**	Based on assumptions in the study by A. Dutta and Phillips (2009)
	SMR duty	MWh/day	1906.30	Calculated using Aspen plus simulation
Water Gas Shift Reactor	Input gas	tonne/day	897.1	Calculated based on mass balance
	Input temperature	°C	315	A. Dutta and Phillips (2009)
	Pressure	kPa	2600	A. Dutta and Phillips (2009)
	Catalyst (copper-zinc-Alumina)	tonne	8.4**	A. Dutta and Phillips (2009)
	Steam	tonne/day	403.26	Calculated based on mass balance
Pressure Swing Adsorption	Temperature of input	°C	25	Swanson et al. (2010)
	Pressure of input	kPa	2500	Swanson et al. (2010)
	PSA booster compressor Power	MWh/day	6.74	Calculated based on mass balance
	Hydrogen output	tonne/day	146.78	Calculated based on mass balance
	Bed material	tonne	111.3**	A. Dutta and Phillips (2009
Hydrogen Compression	Input temperature	°C	50	Based on thermodynamics calculations
	Input pressure	kPa	2500	Based on thermodynamics calculations
	Output temperature	°C	312	Based on thermodynamics calculations
	Output pressure	kPa	20000	Based on thermodynamics calculations
	Power consumption	MWh/day	151.7	Based on thermodynamics calculations
	Isentropic efficiency		81%	The average efficiency for a compressor Campbell (2014, 2015)
Hydrogen Cooling	Output temperature	°C	25	Assumed
	Cooling duty	MWh/day	171.8	Calculated using Aspen plus simulation

* Replaced every 2 years

** Replaced every 3 years

6.3 Inventory datasets

6.3.1 Review of existing hydrogen production inventory datasets in literature

A review was performed for steam methane reforming (SMR) pathways for hydrogen production. There were 6 inventory datasets for SMR, with varying level of details with respect to input and output flows. The following data was collected during the literature review of inventory datasets.

i. Input flows and values
ii. Output flows and values
iii. Functional unit
iv. Background system database references
v. Data quality

Table 6-3 shows the key parameters of SMR hydrogen production pathway including range of reported values and calculated averages. For example, reported natural gas consumption is in the range of 141-165 MJ per 1 kg of H_2 production while the CO_2 emissions of the pathway is in the range of 7.74-12.6 kg per 1 kg of H_2 production.

Table 6-3: Overview of critical parameters of natural gas steam methane reforming life cycle inventory based on literature review (Al-Qahtani, Parkinson, Hellgardt, Shah, & Guillen-Gosalbez, 2021b; Antonini et al., 2020; A. Mehmeti, A. Angelis-Dimakis, G. Arampatzis, S. McPhail, & S. Ulgiati, 2018; Salkuyeh, Saville, & MacLean, 2018; Siddiqui & Dincer, 2019; Sidique, 2010; A. Valente et al., 2020)

Parameter	Range	Average
Natural gas consumption (MJ/1 kg of H_2)	141-165	147
Electricity consumption (kWh/1 kg of H_2)	0.31-2.49	1.8
Water consumption (kg/1 kg of H_2)	7.5-21.9	17.1
CO_2 emissions (kg/1 kg of H_2)	7.74-12.6	9.6
Nitrogen oxide emissions (g/1 kg of H_2)	0.04-11.8	5.8
CO emissions (g/1 kg of H_2)	0.04-8.9	4.8
CH_4 emissions (g/1 kg of H_2)	0.04-42	18.3

6.3.2 Compiling a list of input and outputs flows

The first step of creating a life cycle inventory is to create a list of potential inputs and outputs related to the unit process under study. The list of inputs and outputs for SMR unit process is illustrated in Table 6-4 this list was collected during the literature review.

Table 6-4: List of inputs, outputs and corresponding background database processes/elementary flows reported in the literature for hydrogen production using natural gas steam methane reforming inventory

Flow name	Flow type	Background database process
Input flows		
Natural gas	Technosphere	market group for natural gas, high pressure - EcoInvent
Water	Technosphere	market for water, deionized, from tap water, at user - EcoInvent
Electricity	Technosphere	electricity production, hydro, reservoir, alpine region - EcoInvent
Liquid storage tank, chemicals, organics	Technosphere	market for liquid storage tank, chemicals, organics - EcoInvent
Chemical factory, organics	Technosphere	chemical factory construction, organics – EcoInvent
Aluminum oxide	Technosphere	market for aluminum oxide – EcoInvent
Molybdenum trioxide	Technosphere	market for molybdenum trioxide – EcoInvent
Zinc oxide	Technosphere	market for zinc oxide – EcoInvent
Quicklime, milled, packed	Technosphere	market for quicklime, milled, packed – EcoInvent
Silica sand	Technosphere	market for silica sand – EcoInvent
Chromium oxide, flakes	Technosphere	market for chromium oxide, flakes – EcoInvent
Copper oxide	Technosphere	market for copper oxide – EcoInvent
Magnesium oxide	Technosphere	market for magnesium oxide – EcoInvent
Portafer	Technosphere	market for portafer – EcoInvent
Nickel, 99.5%	Technosphere	market for nickel, 99.5% - EcoInvent
Zeolite, powder	Technosphere	market for zeolite, powder - EcoInvent
Water	Elementary	-
Output flows		
Hydrogen	Reference product	-
Carbon dioxide, fossil	Elementary	-
Black carbon	Elementary	-
Carbon dioxide, from soil or biomass stock	Elementary	-
Acetaldehyde	Elementary	-

Acetic acid	Elementary	-
Benzene	Elementary	-
Benzo(a)pyrene	Elementary	-
Butane	Elementary	-
Carbon monoxide, fossil	Elementary	-
Dinitrogen monoxide	Elementary	-
Formaldehyde	Elementary	-
Mercury	Elementary	-
Methane, fossil	Elementary	-
Nitrogen oxides	Elementary	-
PAH, polycyclic aromatic hydrocarbons	Elementary	-
Particulates, < 2.5 um	Elementary	-
Particulate > 10 um	Elementary	-
Pentane	Elementary	-
Propane	Elementary	-
Propionic acid	Elementary	-
Sulfur dioxide	Elementary	-
Toluene	Elementary	-
Volatile organic compounds	Elementary	-

6.3.3 Life cycle inventory based on process simulation data and interim quality control

Table 6-5 shows the unit process LCI generated for SMR process listing inputs and outputs, quantities values, units and any data treatments applied in calculation. It should be noted that values presented in Table 6-5 represents corrections after a first quality control to identify significant issues including:

i. Removal of unreacted methane by combustion to generate energy for SMR process. Methane emissions are highly sensitive to the global warming impact and it is highly unlikely that any significant methane emitted to the atmosphere, also evidenced by methane emissions values reported in literature (Table 6-3).
ii. System of SMR process was expanded to include heat generation by combustion of natural gas and to include preliminary heat integration, which improves efficiency of the process.

Since no operational data from industrial scale SMR H_2 production is accessible, the current inventory data was compared with literature reported values. For example, the natural gas input and CO_2 emission output of the SMR inventory are within the range of values reported in the literature. The geographical consistency has been maintained by matching the natural gas composition to marketable natural gas available in Alberta. Technological and time-related representativeness of the process, which is based on unit operations reported by NREL report (A. Dutta, and Phillips, S.D., 2009), however can be improved in the future iterations.

A major discrepancy of the current inventory is the lack of many output flows compared to what has been reported in the literature. They include mainly aromatic compounds, heavy metals and particulates. However, such outputs can be neglected in the current study as they do not directly affect the global warming potential impact category.

Table 6-5: Life cycle inventory of hydrogen production using natural gas steam methane reforming unit process, calculated based on process simulation results

Flow name	Value	Unit	Data treatment/assumptions/comments
Input flows			
Natural gas, AB	3.93E+00	m^3	Density = 0.717 m3/kg; Natural gas as feedstock + supplemented as energy source for combustion of off-gases + Theoretical Natural Gas required for steam generation (Result of simulation by CE-V. Same Enbridge natural gas composition was used).
Electricity, AB	1.31E+00	kWh	AB electricity mix 2020, Power consumption MEA unit (40.12 MWh/d), Power consumption air separation unit (0.03 MWh/d) based on assumptions in NREL report. Power consumption MP compressor (185 MWh/d)
Process water	5.09E+00	kg	Deionized water is used for steam generation
Monoethanolamine	3.41E-04	kg	Chemical solvent-based (monoethanolamine, MEA) extraction of sulphur components, based on assumptions in NREL report
Zinc oxide	3.36E-04	kg	Catalyst desulphurization; 36 t replenished every 2 years, based on assumptions in NREL report
Zinc oxide	2.35E-05	kg	Cu-Zn-Al catalyst in the water gas shift reactor; 8.40 metric-tonne replenished every 3 years: composition (%mass): 40% copper oxide, 45% zinc oxide; 15% alumina oxide
Aluminum oxide	7.84E-06	kg	Cu-Zn-Al catalyst in the water gas shift reactor; 8.40 metric-tonne replenished every 3 years: composition (%mass): 40% copper oxide, 45% zinc oxide; 15% alumina oxide
Copper oxide	2.09E-05	kg	Cu-Zn-Al catalyst in the water gas shift reactor; 8.40 metric-tonne replenished every 3 years: composition (%mass): 40% copper oxide, 45% zinc oxide; 15% alumina oxide
Cobalt oxide	2.05E-05	kg	Co_2O_3 catalyst in SMR reactor, 3.29 t replenished every 3 years
Activated carbon	6.92E-04	kg	Molecular sieve is pressure swing absorption bed component: activated carbon; 111.3 t replenished every 2 years, based on assumptions in NREL report
Output flows			
Hydrogen	1.00E+00	kg	146.78 t/d, purity: 99.9%, pressure: 200 bar
Carbon dioxide	1.05E+01	kg	SMR Heater off gas
Sulphur	1.23E-03	kg	Sulphur cake from Air separation + LO-CAT process. Patented H2S to sulfur conversion.
Wastewater	6.81E-07	m^3	Wastewater from Air separation + LO-CAT process. Patented H2S to sulfur conversion.
Water	4.97E+00	m^3	
Nitrogen	2.64E+01	kg	Dry air is used for combustion, so nitrogen is the dominant compound in the final off gases
Oxygen	1.42E+00	kg	20% extra air used for combustion
Sulfur dioxide	2.58E-04	kg	
Nitrogen dioxide	3.48E-05	kg	
Nitric oxide	4.77E-03	kg	
Methane, fossil	0.00E+00	kg	80% conversion; Methane is completely combusted

6.3.4 Addressing data gaps and final life cycle inventories

In SMR unit process inventory, several flows including particulates and volatile organic components were found missing compared to the inventories reported in the literature. However, these flows have no impact in calculation of global warming potential and hence they can be safely neglected. However, these flow should be included in the future, if the analysis is extended to other impact categories such as human health and toxicity.

6.3.4.1 Foreground datasets

Unit process datasets

SMR process (Table 6-6), is presented as unit processes developed in this study. Following data quality naming conventions are used in presented inventory tables.

- Data quality of flows: (Reliability, Completeness, Time related, Geographical, Technological)
- Data quality of process: (Completeness, review)

Table 6-6: Final life cycle inventory of hydrogen production using natural gas steam methane reforming unit process.

Flow name	Value	Unit	Data quality (flows)	Data quality (process)
Input flows				(3,4)
Natural gas, AB	3.93E+00	m^3	(4,1,2,2,1)	
Electricity, AB	1.31E+00	kWh	(3,5,4,3,1)	
Process water	5.09E+00	kg	(3,5,4,3,1)	
Monoethanol amine	3.41E-04	kg	(3,5,4,3,1)	
Zinc oxide	3.36E-04	kg	(3,5,4,3,1)	
Zinc oxide	2.35E-05	kg	(3,5,4,3,1)	
Aluminum oxide	7.84E-06	kg	(3,5,4,3,1)	
Copper oxide	2.09E-05	kg	(3,5,4,3,1)	
Cobalt oxide	2.05E-05	kg	(3,5,4,3,1)	
Activated carbon	6.92E-04	kg	(3,5,4,3,1)	
Output flows				
Hydrogen	1.00E+00	kg	(3,5,4,3,1)	
Carbon dioxide	1.05E+01	kg	(3,5,4,3,1)	
Sulphur	1.23E-03	kg	(3,5,4,3,1)	
Wastewater	6.81E-07	M3	(3,5,4,3,1)	
Water	4.97E+00	m3	(3,5,4,3,1)	
Nitrogen	2.64E+01	kg	(3,5,4,3,1)	
Oxygen	1.42E+00	kg	(3,5,4,3,1)	
Sulfur dioxide	2.58E-04	kg	(3,5,4,3,1)	
Nitrogen oxides	3.48E-05	kg	(3,5,4,3,1)	
Nitric oxide	4.77E-03	kg	(3,5,4,3,1)	
Methane, fossil	0.00E+00	kg	(3,5,4,3,1)	

Aggregated process datasets

Following the announcement in December 2018 of Canadian regulations to phase out traditional coal-fired electricity by 2030 (Canada, 2021), it was essential to have the most up-to-date data regarding the electricity production mix in Alberta since it may change quickly because coal used to have an important is assumed that it has not changed significantly between 2019 and 2020.

The EcoInvent database used in this project was updated to version 3.8, which allegedly contains updated, attributional electricity markets for Canada with a reference year of 2019, rather than 2018 for the previous version (Moreno Ruiz et al., 2021), as shown in Table 6-7. However, the data did not correspond perfectly to the one provided by the Alberta Electric System Operator (AESO), who manages the provincial power grid and had daily data up to 2021.

Table 6-7: Alberta's electricity production mix in 2019 according to Ecoinvent v3.8

Ecoinvent flow	2019 Share
Lignite	47.56%
Natural gas, conventional	32.03%
Co-generation, natural gas	8.99%
Wind, 1-3MW turbine	6.97%
Hydro, reservoir	2.32%
Hydro, run-of-river	1.19%
Co-generation, woodchips	0.67%
Wind <1MW turbine	0.24%
Oil	0.02313%
Wind, >3MW turbine	0.00622%
Co-generation, oil	0.00011%
Co-generation, biogas	0.00001%
TOTAL	**100%**

To be able to use the detailed and connected flows in Ecoinvent, and to run the assessment with the most recent yearly data (2020) from AESO, some data manipulations have been done.

First, using AESO's data, the utilized MWh in Alberta were summed by energy source and the shares of each source in the 2020 power grid were calculated, as shown in Table 6-8.

Then, in Table 6-9, the larger energy sources from AESO in Table 6-8 were broken down into subcategories using the corresponding flows from Ecoinvent in Table 6-7. The shares of the subcategories in the larger energy source were calculated with the data from Table 6-7 as well. It may be noticed in Table 6-9 that the wind energy has not been broken down into the three wind energy flows from Table 6-7. In fact, wind energy is 100% produced by turbines with a capacity that is over 3 MW(AESO, 2022b). Thus, flows for wind energy from <1 MW turbines and 1 to 3 MW turbines were removed from the electricity production mix.

Finally, as shown in Table 6-9, the total shares in 2020 of the subcategories into the larger energy source were obtained by multiplying the 2019 shares by the utilized MWh in 2020. It must be noted that it was assumed that the production mix would not have changed significantly the year from 2019 to 2020.

Table 6-8: Alberta's power grid in 2020 (AESO, 2022a)

Energy source	Subcategory	Produced (MWh)	2020 Share
Coal		20,163,997.64	35.1%
Cogeneration		13,795,425.75	24.0%
Natural Gas		12,539,341.46	21.8%
	Combined cycle	10,085,549.61	17.5%
	Simple cycle	2,453,791.85	4.3%
Wind		6,079,436.99	10.6%
Dual Fuel		2,243,263.42	3.9%
Hydro		2,035,266.86	3.5%
Other		569,693.79	1.0%
Solar		86,270.96	0.2%
Storage		73.90	0.0%
	TOTAL	**57,512,770.77**	**100%**

Table 6-9: Calculations for Alberta's production mix in 2020

AESO energy source	Ecoinvent categories	Shares in energy source in 2019	Produced (MWh) in 2020	Total share in 2020
Coal		**Shares in coal in 2019**	**20,163,997.64**	**35.465%**
	Lignite	100%	20,163,997.64	35.465%
Cogeneration		**Shares in cogeneration in 2019**	**13,795,425.75**	**24.263%**
	Co-generation, natural gas	93%	12,842,837.14	22.588%
	Co-generation, woodchips	7%	952,421.62	1.675%
	Co-generation, oil	0.00114%	157.19	0.00028%
	Co-generation, biogas	0.00007%	9.81	0.00002%
Natural Gas		**Shares in natural gas in 2019**	**12,539,341.46**	**22.054%**
	Natural gas, conventional	20%	2,453,791.85	4.316%
	Natural gas, combined cycle	80%	10,085,549.61	17.739%
Wind		**Shares in wind in 2019**	**6,079,436.99**	**10.693%**
	Wind, >3MW turbine	100.00000%	6,079,436.99	10.693%
Dual Fuel		**Shares in dual fuel in 2019**	**2,243,263.42**	**3.945%**
	Oil	100%	2,243,263.42	3.945%
Hydro		**Shares in hydro in 2019**	**2,035,266.86**	**3.580%**
	Hydro, reservoir	66%	1,343,298.70	2.363%
	Hydro, run-of-river	34%	691,968.15	1.217%

Applying above data following cradle-to-gate aggregated datasets were generated for Alberta (Table 6-10). Only the cradle-to-gate CO_2 equivalent emissions are reported for simplification.

Table 6-10: The CO_2 equivalent emissions for feedstock production processes.

Aggregated dataset	Cradle-to-gate equivalent CO_{2e} emissions
Electricity production mix, Alberta	0.66 kg eq.CO_{2e}/kWh
Market for electricity, high voltage, Alberta	0.67 kg eq.CO_{2e}/kWh
Natural gas consumption mix, Alberta	0.191 kg eq.CO_{2e}/m^3

6.3.4.2 Background inventory datasets

Ecoinvent background inventory database was used for all other technosphere inputs such as chemicals and materials. Either production or consumption mix market processes were used depending on availability. Following prioritization was used when choosing market average processes.

i. Canada or Canadian provinces geographies
ii. Global geography
iii. Rest of the work geography

The background process names of EcoInvent database with connecting flow names of foreground system processes are given in Table 6-11.

Table 6-11: Flows of foreground system and their corresponding background system processes from EcoInvent database.

Flow name	Background system process
Monoethanolamine	market for monoethanolamine | monoethanolamine {GLO}
Zinc oxide	market for zinc oxide | zinc oxide {GLO}
Aluminum oxide	market for aluminum oxide, metallurgical | aluminum oxide, metallurgical {GLO}
Copper oxide	market for copper oxide | copper oxide {GLO}
Activated carbon	market for activated carbon, granular | activated carbon, granular {GLO}
Wastewater	treatment of wastewater, average, capacity 5E9l/year | wastewater, average {CA-QC}
Steam	steam production, as energy carrier, in chemical industry | heat, from steam, in chemical industry (Swanson et al.)
Nitrogen	market for Nitrogen, liquid (Swanson et al.)
KOH	market for potassium hydroxide | potassium hydroxide {GLO}
Polyacrylic acids	market for Acrylic acid {GLO}
Sulfuric Acid	market for Sulfuric Acid {GLO}
Caustic Soda	market for Caustic Soda {GLO}
Chlorine	market for Chlorine {GLO}

6.4 Life cycle impact assessment

In the life cycle impact assessment (LCIA) phase, the methodology explained in ISO:14067:2018 (ISO, 2018) and ISO:14044:2006 (ISO, 2006b) is applied to quantify the potential carbon intensity of each hydrogen production pathway selected and indicated in section 5.1.3.2.4. The climate change impact of each GHG emitted and removed by the hydrogen production system under study is calculated by multiplying the amount of mass of GHG released or took out by the 100-year GWP given in Table 5-4. Hence, the carbon intensity is the sum of these calculated climate change impacts.

The aggregated climate change impacts related to SMR hydrogen production using natural gas are calculated using the open source software openLCA 1.11.0 © developed by Green Delta. The impact method used to calculate the individual emission flows is IPCC 2013. The CI is calculated as 12.11 kgCO_{2e}/kg hydrogen. Figure 6-4 shows the life cycle GHG emissions of the steam methane reforming pathway from the main input flows to the SMR system boundary. Direct GHG emissions from off-gases of LO_CAT© and PSA processes contributes 86% of the total CI of SMR pathway, meanwhile the life cycle GHG emissions from the electricity consumption in the SMR process and utility natural gas demand as SMR feedstock and input flow for steam production represent 7.2% and 6.5% of the total life cycle emissions, respectively.

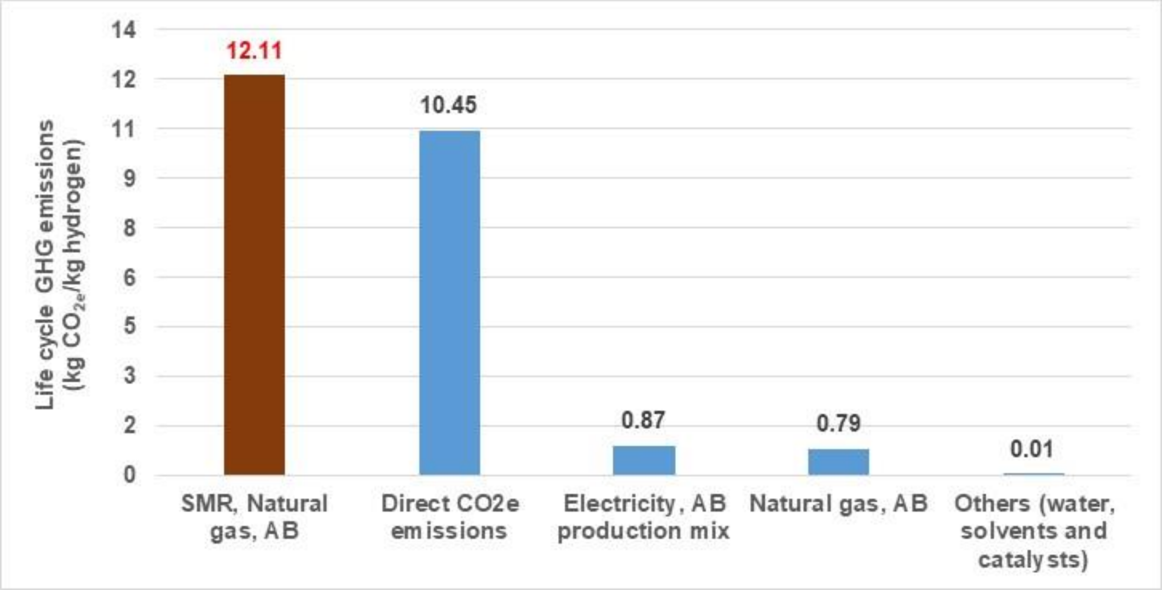


Figure 6-4: Life cycle climate change impacts of hydrogen production using steam methane reforming process with natural gas as feedstock, no CCS, AB

Emissions due to the consumption of electricity production and transmission in the Alberta electricity system account for emissions from Alberta electricity generation mix that depends mostly on fossil fuels electricity generation sources (non-renewable sources). Electricity production from lignite, natural gas, and oil represent 4.1%, 2.5%, and 0.5% of total life cycle GHG emissions of the SMR pathways in AB, respectively (Figure 6-5). The shares of electricity technologies on this market are valid for the year 2020.

Carbon dioxide equivalent emissions from natural gas extraction, production, and transportation represent 1.1%, 1.7% and 2.8% of total CI of SMR pathway in Alberta, respectively (Figure 6-5).

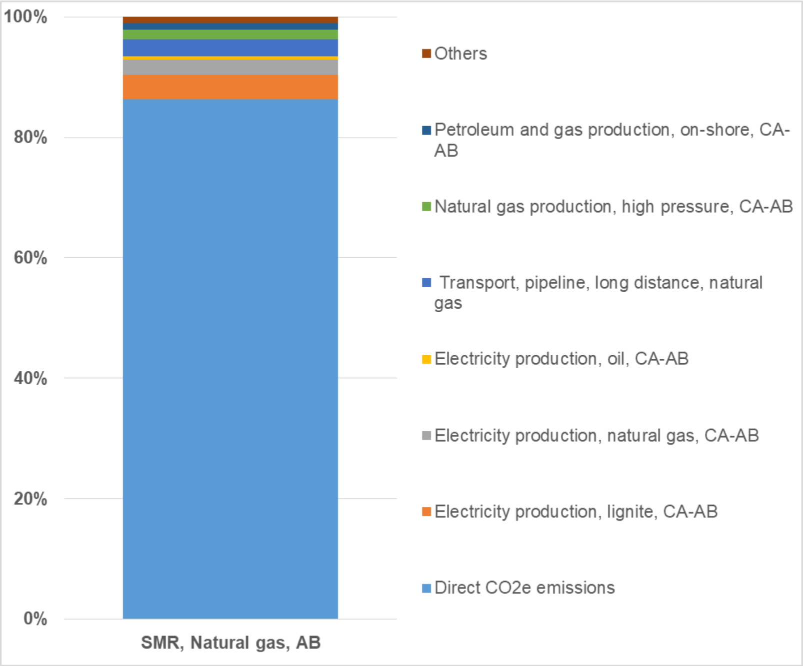


Figure 6-5: Share of life cycle climate change impacts for SMR pathway, natural gas, AB

7 Alkaline Electrolysis Pathway

To have a transition from the conventional steam methane reforming (SMR) generated hydrogen, as described in Sections 6.1and 6.2, to low carbon intensity hydrogen, the hypothetical alkaline electrolysis (AEC) plant requires a large hydrogen production unit at hundreds MW scale. This is much larger than most existing industrial electrolyser demonstration plants, which are typically, at kW or a few MW scale (Chehade, Mansilla, Lucchese, Hilliard, & Proost, 2019). In a large-scale plant, the electrolysis unit is commonly installed in modular configurations, enabling an easy installation as well as a flexible operation according to the demand. The hypothetical AEC plant in this study has a hydrogen production rate of 146.8 tonne/day, same as that from SMR process shown in Section 6, providing 24 hour operation per day.

7.1 System boundary

This section provides a general description of the AEC process system boundary, as shown in Figure 7-1. The purpose of the AEC process is primarily for hydrogen production. The system boundary is formulated in such a way that it can serve as a blueprint, for performing process simulation and establishing the mass balance for the subsequent life cycle environmental impact analysis.

Overall, a harmonized AEC system boundary is illustrated in Figure 7-1, which shows the inputs and outputs flows should be included in this generalized alkaline electrolysis system boundary following the criteria indicated in section 5.1.4. Based on Figure 5-5, the foreground system comprises three subsystems, SS1 that considers the extraction and production of the feedstock, i.e. a water demineralization RO system (SS1a) and electricity production system (SS1b); SS2 focuses on an alkaline electrolyser system; and SS3 that refers to hydrogen compression to obtain hydrogen product that comply with the minimum specifications indicated in Table 5-1.

The alkaline electrolysis system is the core unit of the plant, and requires electricity and deionized water as inputs. High purity deionized water produced by a water demineralization system upstream of the electrolyser is needed to achieve long-term stability. Reverse osmosis (RO) technology is often used in water demineralization process, in which the main operation inputs are electricity and chemicals. In addition to the product of purified water, the remaining brine, which is a mixture of water and solid wastes, has to be discharged. Since the final product from the plant is hydrogen at 200 bar and 25°C with a purity of > 99.9 vol%, as already described in Section 6, this hypothetical hydrogen production plant will be complemented with a compression and cooling step after the electrolyser system.

In addition to the primary product of hydrogen, a significant amount of by-product oxygen is generated in the electrolyser. It can be utilized in some real application scenarios such as those integrating the electrolysis system with an existing host site (e.g. oil refinery, bio refinery producing renewable and sustainable fuels, etc.). However, the recovery of oxygen is out of the work scope of this study, so the oxygen is assumed to be vented directly out to the atmosphere.

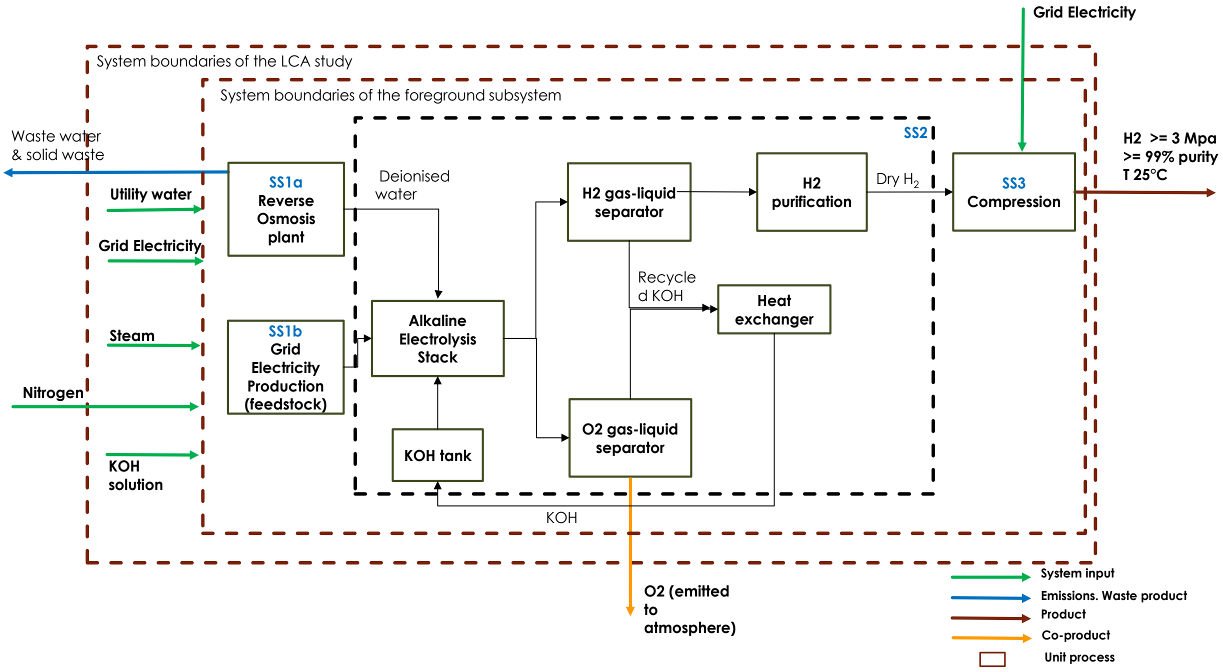


Figure 7-1: System boundary of the alkaline electrolysis pathway.

The production of the input electricity is included in the system boundary. However, its impact on the overall environmental emissions is to be treated in some cases from the background data, depending on the availability of inventory data for specific geographical location and source of the power generation. In the context of this project, Quebec is used as the selected location. The storage, transportation, and utilization of the hydrogen product are out of the work scope.

7.2 Process modelling and simulation

7.2.1 System and process diagram description

To obtain the material and energy flows that are required by the subsequent LCA, a process simulation of the entire process is performed. According to the given system boundary, a process diagram is established designed. The commonly required operation units in AEC industrial plants (Sakas et al., 2022) are considered, and the integrated process diagram is described in Figure 7-2.

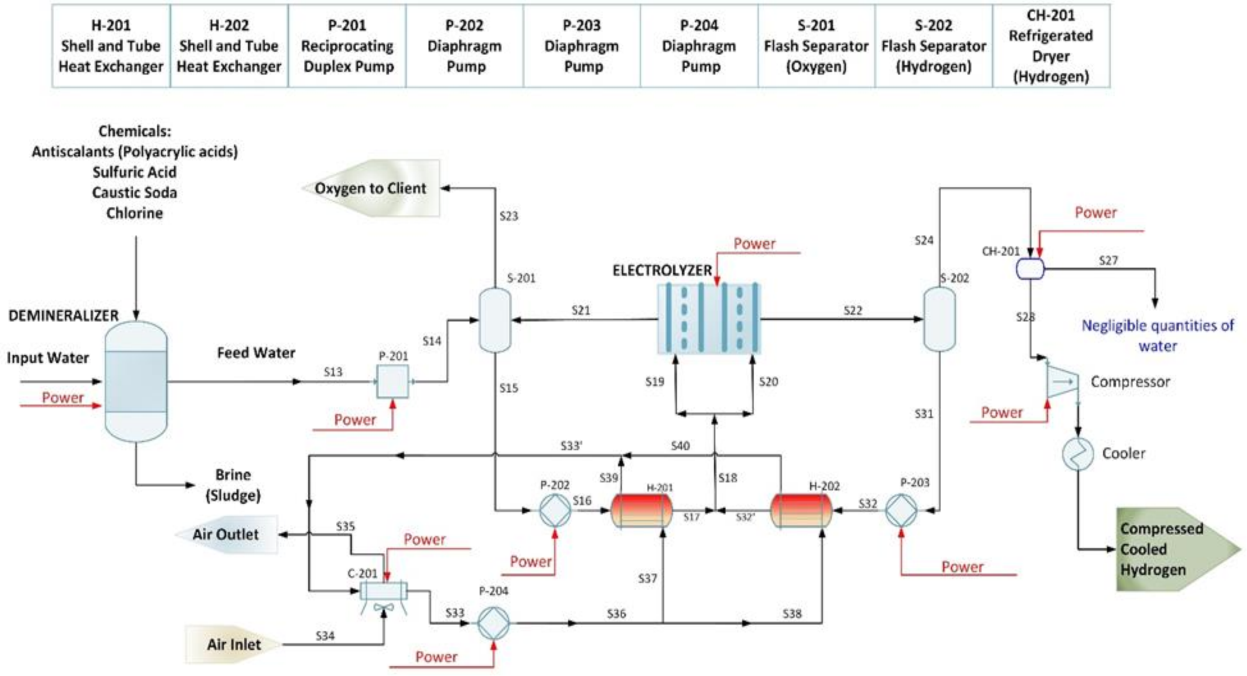
7.2.1.1 Water demineralization

The first step of the process is to obtain the feedstock of deionized water for the electrolysis system, which is done in the demineralization unit, where the reverse osmosis process takes place. Chemicals are needed in the demineralization process, and the electricity consumption is mainly to power the water pump for the uptake of the feed water (Pan, Haddad, Kumar, & Wang, 2020). Minerals are separated from the water together with some of the chemicals and extracted from the system in the brine stream.

7.2.1.2 Alkaline water electrolyser

The alkaline water electrolysis system is made of electrolyser cell stacks and their associated balance of plant units. Electricity is supplied to the electrolyser cell stack through the electrodes, where the water in an electrolyte solution is converted into hydrogen and oxygen through the water-splitting electrochemical reaction, as shown in Eq. (1):

$$H_2O \rightarrow H_2 + \frac{1}{2}O_2 \tag{1}$$



H-201 Shell and Tube Heat Exchanger	H-202 Shell and Tube Heat Exchanger	P-201 Reciprocating Duplex Pump	P-202 Diaphragm Pump	P-203 Diaphragm Pump	P-204 Diaphragm Pump	S-201 Flash Separator (Oxygen)	S-202 Flash Separator (Hydrogen)	CH-201 Refrigerated Dryer (Hydrogen)

Figure 7-2: Schematic process diagram of the alkaline water electrolyser plant.

The mixture of the electrolyte solution and gas molecules of H_2 and O_2 is then directed into two loops. In each loop, a horizontal gravity gas-liquid separator vessel (S-201 / S-202) is used to divide the mixture flow into separate streams.

The separated electrolyte is recirculated back to the cell stack by centrifugal pumps (P-202 and P-203), which serve to control the mass flow rate of the electrolyte and maintain the efficiency of recirculation (Sakas et al., 2022). The electrolyte flowing in the closed loop is cooled down through heat exchangers (H-201 and H-202) before entering the stack. The cooling circuit is composed of an integrated cooling pump (P-204), which directs the cooling water through the heat exchangers to remove the water heat, and an air cooler (C-201), so that the temperature of returned electrolyte is maintained as required in the cells. Before returning to the cell stack, the cathode and anode electrolyte streams are mixed, which could potentially increase the occurrence of gas impurities (Brauns & Turek, 2020; P. Trinke3, Brauns, Bensmann, Hanke-Rauschenbach, & Turek, 2018).

The hydrogen flow after the gas-liquid separator enters a purification system (CH-201) to remove the moisture, or even the O_2 residuals if there is any to create a high-quality dry hydrogen gas flow. The purified hydrogen gas out of the purification process is ready to be compressed and stored. On the other side of the electrolyser, the oxygen stream normally undergoes a similar purification process if it is to be recovered. As mentioned, in this study, oxygen is assumed to be vented to the atmosphere directly after the gas-liquid separation process without going through the purification step.

7.2.1.3 Compression

As the final step (see Figure 7-2), the pure and dry hydrogen gas flow is delivered to be compressed and cooled down. The purpose of this compression step is for the hydrogen stream to reach a uniformed state (200 bar and 25°C), as from other technologies (e.g. Steam methane reforming). The consistency of the final product state allows for a fair comparison of the LCA study results. The final pressure of the hydrogen before storage is dependent on the subsequent applications.

7.2.2 Input assumptions

To establish the overall mass balance data of the plant for use in the upcoming LCA study, the process simulation is carried out with I-BIOREF software platform, which includes comprehensive chemical process analysis in the context of decision making. Description of I-BIOREF software platform (NRCan, 2015) can be found in Appendix 9. The modeling of the electrolysis itself is based on kinetic modeling for the calculation of cell potential according to the Ulleberg method using semi-empirical equations (Ulleberg, 2003). The specifications and input assumptions for the process simulations are introduced below.

The alkaline water electrolyser stacks operating at 30 bar and 75 °C was simulated based on a typical operating pressure of large MW scale electrolysers (McPhy, 2022; Navarro, Guil, & Fierro, 2015). Currently, the electrolyser modules in the market can range from 100 to 800 Nm^3/h (McPhy, 2022), which is roughly about the power capacity of 0.5-4 MW. To have the similar hydrogen production capacity as the SMR process (146.8 tonne/day), the AEC plant requires a high number of stacks. In the modeling of the electrolyser, we assume the active electrode area of 3 m^2 for each stack and each stack has a maximum power capacity of 2.2 MW (Nel, 2022) consisting of 200 cells. To reach the targeted hydrogen production rate of 146.8 tonne/day, the simulation showed that 152 electrolyser stacks of 2.2 MW/stack are needed. The overall power capacity of the plant is 334.0 MW, corresponding to the energy consumption of 54.6 kWh/H_2. These technical characteristics of the electrolysis system are listed in in Table 7-1.

Table 7-1: AEC process simulation specifications and input assumptions.

Parameter	Value	Unit	Reference
Hydrogen (dry) purity	> 99.9	%	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
Hydrogen (dry) output pressure	200	bar	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
Hydrogen (dry) output temperature	25	°C	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
Hydrogen production rate	146.8	tonne/day	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
Stack working temperature	75	°C	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation

Stack operating pressure	30	bar	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
KOH electrolyte concentration	35	wt%	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
No. of cells per stack	200	-	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
Active electrode area per stack	3	m^2/stack	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
Stack power	2.2	MW/stack	(Nel, 2022)
Recovery rate of brackish RO	70	%	(Sakas et al., 2022)
Electricity consumption for brackish RO water desalination process	1.55	kWh/m^3 deionized water	(Pan et al., 2020)
Adiabatic efficiency of gas-liquid separator	100	%	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
Pressure drop of gas-liquid separator	4	bar	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
Efficiency of heat exchanger	100	%	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
Heat duty of heat exchanger	13.0	MW	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
Isentropic efficiency of pumps	40	%	40% is considered for flow rates below 200 USgpm (Peters, 2020)
Efficiency of air cooler	75	%	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
Pressure drop of air cooler	0.07	bar	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
Air pressure	2	bar	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
Isentropic efficiency of compressor	81	%	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation

Electrolyte KOH concentration in AEC systems may vary from 20 to 40 vol%, and 35 vol% as used in the simulations for this study. All four pumps employed in the electrolyser system are assumed to have an isentropic efficiency of 40% (Peters, 2020). The air cooler has an efficiency of 75% along with a pressure drop of 0.07 bar. The compressor has an isentropic efficiency of 70% based on a typical reciprocating compressor, which is used to calculate its power consumption.

As shown in the process diagram Figure 7-2, the electrolyte is recirculated in the system design and reused in the electrolysis unit. A small amount of KOH solution may be lost over time due to leakage or losses during electrolysis. In reality, there could be a small buffer tank present in the electrolyte recirculation loop, and additional deionized water is added to electrolyte in the buffer tank to replenish. However, in this study we did not consider the KOH loss and so there is no need of replenishment during operation, instead it is assumed that the KOH solution is disposed and completely replaced after 10 years (J. Koj, C. Wulf, A. Schreiber, & P. Zapp, 2017; Koj, Schreiber, Zapp, & Marcuello, 2015).

Depending on the technologies at maturity, O_2 residuals could also be present in the hydrogen gas flow before purification due to two main phenomena: 1) the diffusion of the oxygen product gas through the diaphragm from the anode to the cathode cell; and 2) the dissolution of oxygen gas in the electrolyte circulation from the anode side, which is mixed with the electrolyte circulation from the cathode side before returning to the cell stack, are carried over to the hydrogen stream (Sakas et al., 2022). Similarly, a small fraction of H_2 could also be present in the oxygen by-product stream, which contributes to the total H_2 loss. The removal of O_2 residuals in the H_2 gas stream can be done in a deoxidizer (Sakas et al., 2022), leading to H_2 losses as the result of the recombination reaction to produce water. The total amount of H_2 loss can vary depending on specific technology and its associated maturity level, One glimpse can be seen from the modeling results of AEC process (Sakas et al., 2022), in a steady state, from the produced hydrogen there is a 2.5 % loss into gas impurities due to process mixing and diaphragm diffusion, and a 0.4 % loss in the deoxidizer to purify the hydrogen flow from oxygen residuals. In this study, according to the gathered data for modeling from the providers, the overall H_2 loss due to the above two causes was not considered. Thus, the hydrogen purification process only considers the drying process, assuming there are no O_2 residuals present.

The hydrogen purification system is assumed to be using a refrigerated drying technology. Refrigerated driers act as high-pressure product gas chillers that can condense water out of the product streams. The refrigeration unit operates on a vapor-compression refrigeration cycle, which generally includes an evaporator, compressor, condenser, throttle valve and refrigerant (NRCan, 2021).

Furthermore, air and cooling water are required to flow in the KOH recirculation process for the electrolyte cooling purpose, and the same amounts are assumed to flow out afterwards. As non-consumables, the amount of air and cooling water will not affect the final GHG emission analysis results, and thus their flows were not simulated in the process simulation.

Regarding the generation of deionized water, the RO process was used since it is one of the most common desalination technologies. The energy requirement is highly dependent on the water quality (such as salinity) of the available source, since it mainly comes from the use of high-pressure pumps. The quality of feed water is location-dependent for the real plant. In our study, the plant is assumed to be near a river or lake for an easy access to fresh water and brine discharge, and hence the water is assumed to be brackish water (salinity of 1-15 g/L), and a brackish water RO (BWRO) rather than the seawater RO is considered. The recovery ratio of the water (flow rate ratio of generated clean water to the brackish feed water) by BWRO can range from 50% to 90%, depending on the different configurations adopted (Pan et al., 2020). The average water recovery ratio of 70% was assumed. The energy consumption to produce a unit of deionized water generally can vary from 0.8-2.5 kWh/m^3 based on the review of BWRO plants (Pan et al., 2020). A specific energy requirement of 1.55 kWh/m^3 is assumed for the RO in this AE plant, which is an average value of 1.4 -1.7 kWh/m^3 from a RO process with treatment capacity of 360 m^3/day (Pan et al., 2020) This is the most approximate scale based on the open literature and common practices. As shown in Table 7-2, this corresponds to 0.014 kWh/kg H_2 energy requirement for the RO process, to meet the electrolyser's demand (deionized water of 9.12 kg/kg H_2).

Table 7-2: Technical characteristics of simulated AEC process.

Parameter	Value	Unit	Reference
Electrolyser system power capacity (stacks only)	334.032	MW	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
Electricity consumption (stack only)	54.6	kWh/kg H_2	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
No. of stacks	152	-	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
KOH (35 wt%) quantity in recirculation	0.81	g/kg H_2	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
Electricity/power consumption of auxiliary components			
Pump for deionized water uptake	121.4	kW	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
Pump in cathode electrolyte recirculation	300.6	kW	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
Pump in anode electrolyte recirculation	309.1	kW	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
Pump and fan in cooling loop	182.0	kW	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
Refrigerated dryer for H_2 purification	2933.7	kW	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
Compression of purified H_2	5.03	MW	Chemical process analysis combining Excel-based and I-BIOREF modeling and simulation
RO demineralization	0.014	kWh/kg H2	(Pan et al., 2020)

Based on the above assumptions, the technical characteristics of the modeled AEC process are generated through the process simulation and listed in Table 7-2. It is noted that the quantity of KOH electrolyte (35 vol%) in the recirculation loop is simulated to be 0.81 g/kg H_2.

7.2.3 Mass balance

The mass balance information of the simulated AEC process is summarized in Table 7-3. The power/energy inputs can be found in Table 7-2 above. These will serve as the inputs of the base scenario for the subsequent LCI datasets (see section 7.3). The calculated values are based on mass balances, as well as thermodynamics and kinetics that are all embedded in NRCan's I-BIOREF software.

Table 7-3: Mass balance information of the simulated AEC process in the lifetime of 20 years (146.8 tonne H_2/day).

Parameter	Value	Unit	Comment
Input			
Brackish feed water	1912.4	m^3/day	Salinity within 1-15g/L
Deionized water feed to electrolyser (intermediate input)	9.12	kg/kg H_2	
Total KOH (35 wt.%) quantity requirement	0.81	g/kg H_2	Replaced once in plant lifetime of 20 years
Chemicals for RO desalination			
Antiscalants (Polyacrylic acids)	0.004	tonne/day	(Carollo, 2015)
Sulfuric Acid	0.018	tonne/day	(Carollo, 2015)
Caustic Soda	0.001	tonne/day	(Carollo, 2015)
Chlorine	0.003	tonne/day	(Carollo, 2015)
Output			
Hydrogen production	146.8	tonne/day	-
Oxygen production	1191.3	tonne/day	-
Brine (Water, sulfuric acid, caustic soda, antiscalant, chlorine, salts)	573.72	m^3/day	Calculated based on mass balance

7.3 Inventory datasets

7.3.1 Review of existing hydrogen production inventory datasets in literature

A review was performed for the alkaline electrolysis (AEC) pathway for hydrogen production. There were 7 inventory datasets AEC, with varying level of details with respect to input and output flows. The following data was collected during the literature review of inventory datasets.

i. Input flows and values
ii. Output flows and values
iii. Functional unit
iv. Background system database references
v. Data quality

Table 7-4 shows the key parameters of AEC hydrogen production pathway including range of reported values and calculated averages. The electricity consumption of AEC pathway varies from 50 to 66.2 kWh per 1 kg of H2 production. A fairly large variation in water consumption has been reported from 10 to 19.7 kg per 1 kg of H2 production.

Table 7-4: Overview of critical parameters of alkaline electrolysis life cycle inventory based on literature review (Ghandehariun & Kumar, 2016; J. Koj et al., 2017; Kuckshinrichs & Koj, 2018; D. Ravikumar, Keoleian, G., Miller, S., 2020; Antonio Valente, Diego Iribarren, Javier Dufour, & G. Spazzafumo, 2015; Wulf & Kaltschmitt, 2018b)

Parameter	Range	Average
Water consumption (kg/1 kg of H_2)	10-19.7	13.3
Electricity consumption (kWh/1 kg of H_2)	50-66.2	54.3

KOH consumption (g/1 kg of H_2)	0.27-2.42	1.2
N_2 consumption (g/1 kg of H_2)	0.07-0.29	0.18
Steam consumption (kg/1 kg of H_2)	0.11	0.11
O_2 production (kg/1 kg of H_2)	8.0-8.7	8.4

7.3.2 Compiling a list of input and outputs flows

List of inputs and outputs for AEC unit process is shown inTable 7-5. In contrast to SMR process, AEC literature review did not reveal any specific background system processes. However, EcoInvent database has been reported to be used as background database for AEC process.

Table 7-5: List of inputs, outputs and corresponding background database processes/elementary flows reported in the literature for hydrogen production using alkaline electrolysis inventory

Flow name	Type	Background database process
Input flows		
Electricity	Technosphere	-
Water, deionized	Technosphere	-
Nitrogen	Technosphere	-
Potassium hydroxide	Technosphere	-
Steam	Technosphere	-
Air	Elementary	-
Output flows		
Hydrogen	Reference product	-
Oxygen	Elementary	-
Air	Elementary	-
Effluent waste	Technosphere	-

7.3.3 Life cycle inventory based on process simulation data and interim quality control

Similar to SMR process, LCIs for AEC process was also calculated using the results of process simulation. Two unit processes were defined.

i. Production of deionized water (Table 7-6)
ii. Alkaline electrolysis, purification and compression for hydrogen production (Table 7-7)

Production of deionized water intermediate unit process acts as an input flow for the AEC unit process. The quality control procedure described for SMR process section was also applied to the AEC process. The calculated inventory values for water and electricity consumption is generally in agreement with the literature value reported in Table 7-4. The water consumption is close to the lower end of the range of values obtained from the literature, however, this is arising from consideration of deionized water production and AEC as separate unit processes. A data gap exists in terms of missing flows of N_2 and steam, which is used for the cleaning and start-up of the electrolyser. Since such data cannot be generated from a process simulation, data gap addressing methodology described in section 7.3.4 was used.

Table 7-6: Life cycle inventory of production of deionized water unit process, calculated based on process simulation results.

Flow name	Value	Unit	Data treatment/assumptions/comments
Input flows			
Water	1.43	kg	Water from natural water bodies containing ~8 g/L minerals. Assumed water density of 1000 kg/m^3.
Electricity	0.00155	kWh	
Antiscalants (Polyacrylic acids)	2.70E-06	kg	
Sulfuric Acid	1.35E-05	kg	
Caustic Soda	7.58E-07	kg	
Chlorine	2.16E-06	kg	
Output flows			
Deionized water	1	kg	Assumed water density of 1000 kg/m^3
Brine	0.43	kg	Assumed density of 1000 kg/m^3

Table 7-7: Life cycle inventory of hydrogen production using alkaline electrolysis unit process, calculated based on process simulation results.

Flow name	Value	Unit	Data treatment/assumptions/comments
Input flows			
Electricity	54.61	kWh	Electricity demand for electrolyser stack
Electricity	0.13	kWh	Electricity demand for pumps
Electricity	0.02	kWh	Electricity demand for air cooler
Electricity	0.48	kWh	Electricity demand for H_2 purification
Electricity	0.82	kWh	Electricity demand for H_2 compression
KOH solution (35%)	0.81	g	Calculated assuming this amount of KOH will be completely replaced in 10 yrs. and plant lifetime plant of 20 years.
Deionized water	9.12	kg	Deionized water production unit process is given in Table 7-6
Output flows			
Hydrogen	1	kg	Total flow: 146.8 mt/d, purity: 99.998%, pressure: 200 bar
Oxygen	8.115	kg	

7.3.4 Addressing data gaps and final life cycle inventories

In AEC unit process dataset, the missing flows of steam and nitrogen inputs however affect the global warming impact. Hence, the quality of literature available data was assessed. Among the multiple references to steam and N_2 quantities, the values reported by Kuckshinrichs and Koj (2018) were the most recent and was based on pilot plant data, which provides higher DQI indicator score in terms of reliability. Hence, missing flows were addressed using values reported by Kuckshinrichs and Koj (2018). Also, addressing the missing flows in AEC dataset improved the process completeness DQI.

7.3.4.1 Foreground inventory datasets

Unit process datasets

AEC process (Table 7-8) and deionized water production (Table 7-9) are presented as unit processes developed in this study. Following data quality naming conventions are used in presented inventory tables.

i. Data quality of flows: (Reliability, Completeness, Time related, Geographical, Technological)
ii. Data quality of process: (Completeness, review)

Table 7-8: Final life cycle inventory of hydrogen production using alkaline electrolysis unit process

Flow name	Value	Unit	Data quality (flows)	Data quality (process)
Input flows				(2,4)
Electricity	54.61	kWh	(2,5,3,2,1)	
Electricity	0.13	kWh	(2,5,3,2,1)	
Electricity	0.02	kWh	(2,5,3,2,1)	
Electricity	0.48	kWh	(2,5,3,2,1)	
Electricity	0.82	kWh	(2,5,3,2,1)	
KOH solution (35%)	0.81	g	(2,5,3,4,1)	
Deionized water	9.12	kg	(3,1,1,3,1)	
Steam	0.04	kg	(2,5,3,4,1)	
Nitrogen	0.71E-4	kg	(2,5,3,4,1)	
Output flows				
Hydrogen	1	kg	(2,2,3,2,1)	
Oxygen	8.115	kg	(2,2,3,2,1)	

Table 7-9: Final life cycle inventory of deionized water production unit process

Flow name	Value	Unit	Data quality (flows)	Data quality (process)
Input flows				(3,4)
Water	1.43	kg	(3,1,1,3,1)	
Electricity	0.00155	kWh	(3,1,1,3,1)	
Antiscalants (Polyacrylic acids)	2.70E-06	kg	(3,1,1,3,1)	
Sulfuric Acid	1.35E-05	kg	(3,1,1,3,1)	
Caustic Soda	7.58E-07	kg	(3,1,1,3,1)	
Chlorine	2.16E-06	kg	(3,1,1,3,1)	
Output flows				
Deionized water	1	kg	(3,1,1,3,1)	
Brine	0.43	kg	(3,1,1,3,1)	

Aggregated process datasets

The electricity production and market for electricity datasets of Quebec are reported unchanged from the EcoInvent database (Table 7-10). Only the cradle-to-gate CO_2 equivalent emissions are reported for simplification.

Table 7-10: The CO_2 equivalent emissions for feedstock production processes.

Aggregated dataset	Cradle-to-gate equivalent CO_{2e} emissions
Electricity production mix, Quebec	0.015 kg eq.CO_{2e}/kWh
Market for electricity, high voltage, Quebec	0.024 kg eq.CO_{2e}/kWh

7.3.4.2 Background inventory datasets

Same information as in section 6.3.4.2.

7.4 Life cycle impact assessment

Following the same criteria to perform LCIA used for the SMR use case in section 6.4. The carbon intensity of the alkaline electrolysis hydrogen production pathway is calculated as 1.37 kg CO_{2e}/kg H_2. Figure 7-3 indicates the life cycle GHG emissions of alkaline electrolysis pathway from the main input flows to the AEC system boundary. Figure 7-4 illustrates the contribution of feedstock and other materials inputs flows to the overall life cycle climate change impact of AEC pathway. Life cycle GHG emissions of electricity from the QC electricity grid system represents 99 % of the total CI of AEC pathway, meanwhile the 1 % is mostly related to the steam and KOH electrolyte solution inputs flows. Electricity demand for the electrolyser stack usage represents 97% of total electricity input.

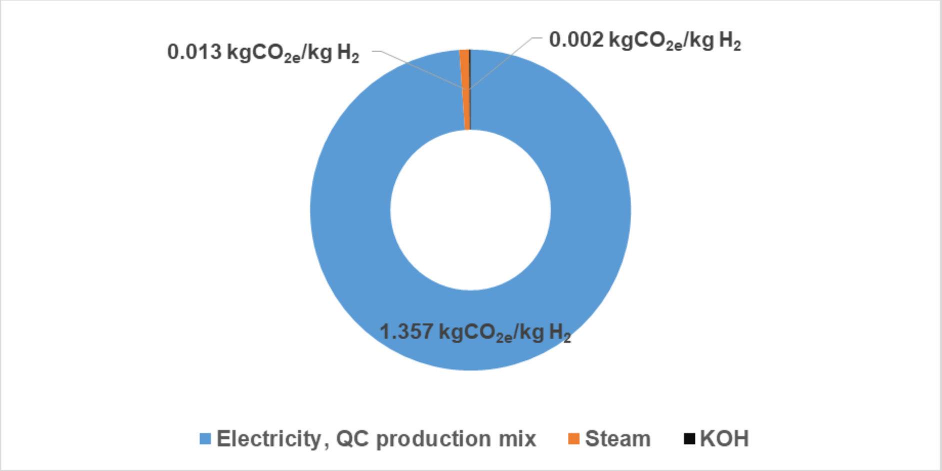


Figure 7-3: Life cycle climate change impacts of hydrogen production using alkaline electrolysis and QC grid electricity as feedstock.

Emissions due to the consumption of electricity production and transmission in the Quebec electricity system account for emissions from the Quebec electricity generation mix, electricity imports, and electricity transmission as greenhouse gas nitrous oxide formation due to ionisation of air molecules and transmission grid losses, which represent 54%, 34%, and 7%, respectively. The shares of electricity technologies on this market are valid for the year 2019.

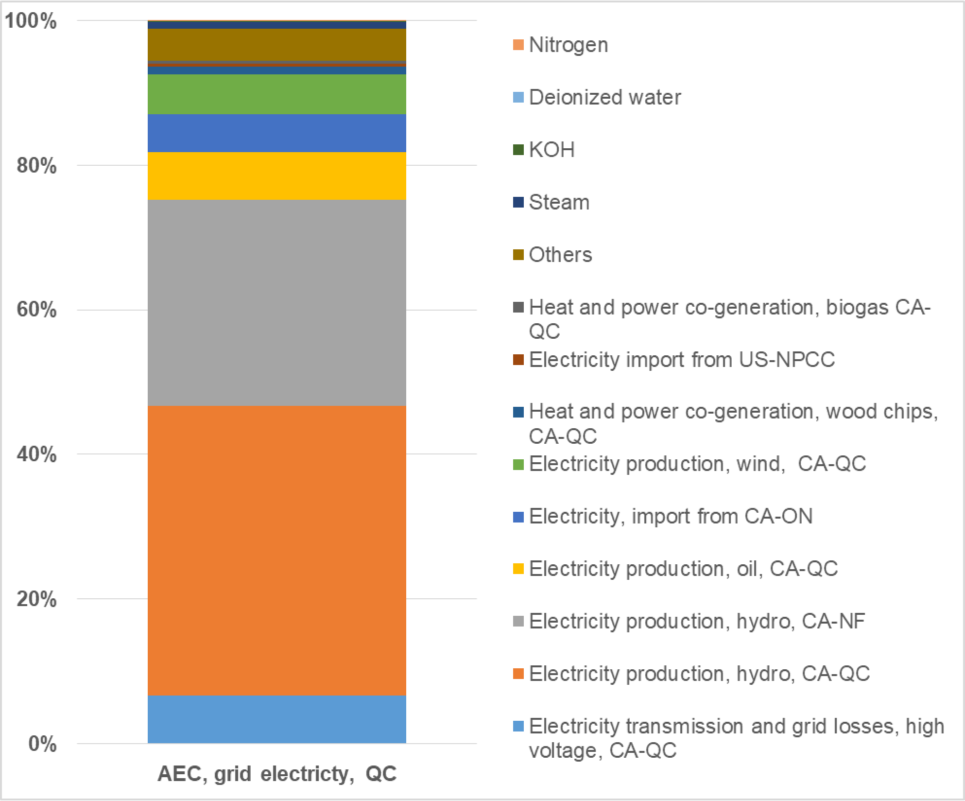


Figure 7-4: Share of life cycle climate change impacts for AEC pathway, grid electricity, QC

Figure 7-5 shows the breakdown of carbon intensities from renewable sources in the AEC pathway in QC. Emissions from renewable sources represent 86% of total carbon intensity of alkaline electrolysis pathway to produce hydrogen in Quebec, Canada. Emissions from hydroelectricity, wind, and biomass production represent 70%, 6%, and 1.3%, respectively.

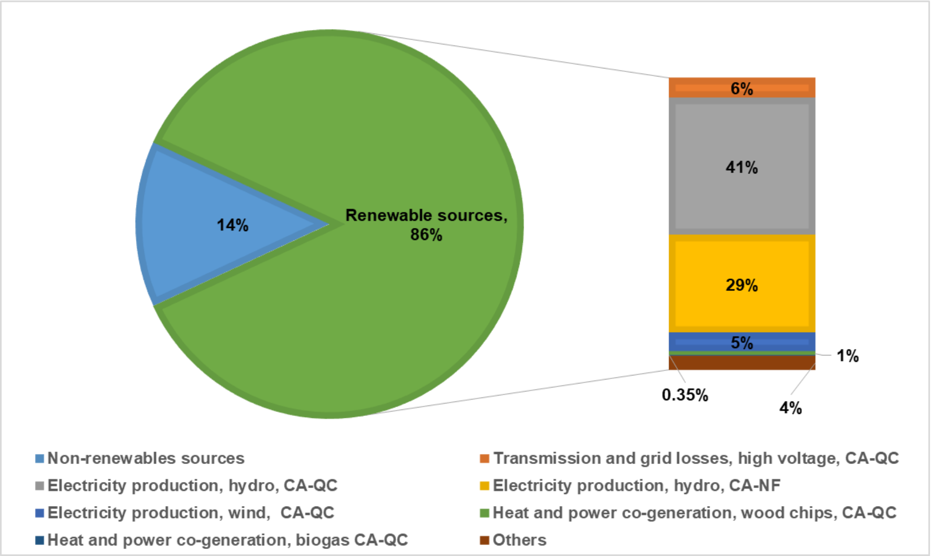


Figure 7-5: Breakdown of carbon intensities from renewable sources in the AEC pathway in QC

8 Discussion and Conclusions

8.1 Discussion

This life cycle assessment study set out the goal of quantifying the carbon intensity of hydrogen production pathways within a Canadian context. Steam methane reforming process is identified as a baseline pathway to be compared with the remaining hydrogen pathways selected in this study.

Figure 8-1 shows the comparison between the calculated carbon intensity of SMR and AEC pathways in Canada and the adopted low-carbon carbon intensity threshold from CertifHy, an EU-wide Guarantee of Origin scheme for green and low carbon hydrogen that considers both the origin of the hydrogen and its carbon intensity, which is 36.4 $kgCO_{2e}$/ MJ $H_{2.}$ This value is set at a 60% below the intensity of the best available technology, i.e. hydrogen produced from natural gas (CertifHy, 2019). In the case of Canada, the hydrogen production from natural gas is assumed to be an SMR process using utility natural gas as feedstock and without CCS in the province of Alberta. Hence, a potential threshold to achieve low-carbon intensity of hydrogen production would be 40.4 $kgCO_{2e}$/ MJ H_2 (4.84 $kgCO_{2e}$/ kg H_2), set at least 60% less emissions than hydrogen baseline pathway and using a lower heating value =119.9 MJ/kg of H_2. All the hydrogen production pathways below this estimated threshold would be eligible to be identified/certified as low-carbon hydrogen.

There are two factors that need to be addressed to achieve low-carbon hydrogen, the amount of renewable energy sources used to produce hydrogen, especially by processes using multiple energy inputs, and the minimum carbon intensity target that hydrogen technology pathways should achieve using renewable and non-renewable energy sources.

Further work on carbon intensity of hydrogen pathways is still needed. Since a wide range of hydrogen pathways from different energy sources can be assessed to define and quantify their CIs and establish thresholds to be independently certified.

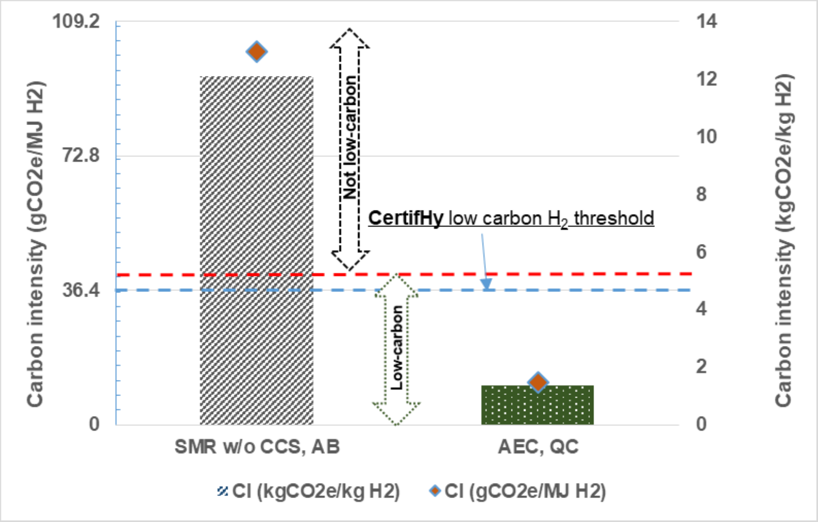


Figure 8-1: Carbon intensities of hydrogen from hydrogen production pathways, SMR and AEC in Canada

Note that all the GHG emissions generated in both hydrogen production pathways studied are allocated to hydrogen product. SMR simulation design considers no excess of steam production, an SMR co-product. In the case of alkaline electrolysis process, oxygen is co-produced to hydrogen in the electrolysis process. Regardless of the technical feasibility of further utilization of oxygen, GHG emissions are not allocated to oxygen product in this study as there is not an adequate allocation procedure for hydrogen and oxygen.

8.2 Conclusions and recommendations

Overall, in this life cycle assessment of hydrogen production pathways study, a scoping review of relevant hydrogen LCA studies was conducted to support the development of a harmonized LCA-based methodology to quantify the carbon intensity of hydrogen production pathways in a Canadian context. Methodology based on ISO 14040/44/67 standards and other protocol documents that should be aligned to current global hydrogen certification and guarantee of origin processes that facilitate the international tradability of hydrogen. Two pathways were evaluated with the LCA-based methodology, SMR using natural gas in Alberta and alkaline electrolysis using grid electricity in Quebec. SMR pathway is assumed as the baseline pathway that would facilitate a classification of carbon intensity of hydrogen production pathways, based on an emission intensity threshold, for certification of hydrogen. The quantification of life cycle carbon intensities of SMR and AEC hydrogen pathways in Canada lead to the following conclusions:

Under the umbrella of a comprehensive and robust methodological framework based on life cycle assessment for hydrogen production systems, the definition of harmonized LCA elements such as functional unit, system boundaries, and co-products allocation facilitates the decision-making for hydrogen suppliers related to participate in hydrogen certification of origin schemes in Canada.

It is confirmed that a substantial dependency of most GHG emissions results on hydrogen production phase, especially from off-gases generated in LO-CAT© and PSA processes and electricity supply in the SMR and AEC pathways, respectively.

The use of non-renewable energy sources as feedstock in the steam methane reforming pathway represents the most important GHG emissions contribution of the total carbon intensity quantified for SMR process in Alberta, hence carbon capture and sequestration can be justified from a GHG emissions reduction and low carbon intensity hydrogen perspective.

The alkaline electrolysis pathway indicates that different levels of low carbon intensity would depend on the renewable sources contribution in the power generation mix of the grid electricity system where the hydrogen production facility is located. Supplied electricity from the grid can have a large extent of different climate change impacts using province-specific electricity mixes in Canada.

Uncertainties of carbon intensity results under a life cycle approach depend on the quality of life cycle inventory data available. A complete and exhaustive revision of the data quality used in the foreground system is needed to assure a representative carbon intensity value for the hydrogen production pathway evaluated.

Recommendations related to methodology of quantifying and classifying GHG emissions of hydrogen production pathways for certification of hydrogen are as follows:

This LCA-based methodology for hydrogen production pathways and carbon intensity quantification should be subject to a critical review performed by experts in the LCA field to endorse if the presented methodology is consistent with ISO 14040/44/67 standards.

Allocation of co-products were not used in this study, however, further research on multifunctional allocation procedures is needed to classify carbon intensity with accuracy.

Building synergies with other clean fuel life cycle assessment tools developed in Canada and/or North America to harmonize approaches to quantify carbon intensity of hydrogen production pathways.

Performing interviews with industry experts and policy leaders to explore the potential of harmonizing approaches across Canada to align and scale efforts in the adoption of national definitions and standards for quantification of carbon intensity of different hydrogen production pathways as well as classification of low carbon intensity hydrogen.

9 Appendix

9.1 Literature reviewed for LCA methodologies on hydrogen production

Item #	Geographical region	Functional unit	Final Pressure of H2	System boundary	Multifunctionality	Primary data	LCIA Method	Impact categories	Reference
1	Others (Brazil)	kg H2	-	Cradle-to-grave	-	No	ReCiPe	GWP & others	(Velandia Vargas & Seabra, 2021)
2	USA	MJ H2	-	Cradle-to-grave	-	No	IPCC	GWP	(Isaacs et al., 2021)
3	USA (California)	kg H2	-	Cradle-to-grave	-	No	IPCC	GWP	(Sinha & Brophy, 2021)
4	-	kg H2	-	Cradle-to-gate	(mass, energy, market value) allocation; and system expansion (Oxygen)	Partial (process simulation)	-	GWP	(Motazedi, Salkuyeh, Laurenzi, MacLean, & Bergerson, 2021)
5	Europe (Netherlands)	kg H2	-	Cradle-to-gate	-	Partial (technology analysis)	ILCD	GWP & others	(Delpierre, Quist, Mertens, Prieur-Vernat, & Cucurachi, 2021)
6	Europe (UK)	MW_HHV H2	300 bar	Cradle-to-gate	Substitution (electricity)	Partial (real plant)	EF 3.0 (GaBi)	GWP & others	(Amaya-Santos et al., 2021)
7	USA	kg H2	-	Cradle-to-gate	-	No	ReCiPe	GWP & others	(Al-Qahtani, Parkinson, Hellgardt, Shah, & Guillen-Gosalbez, 2021a)
8	Europe (Spain)	kg H2	-	Cradle-to-gate	-	No	IPCC	GWP	(Antonio Valente, Diego Iribarren, & Javier Dufour, 2020)
9	Europe (France)	kg H2	-	Cradle-to-gate	-	No	ReCiPe	GWP & others	(Sharma et al., 2020)
10	Others (Iran)	kg H2	-	Cradle-to-gate	-	No	IPCC	GWP & others	(Sadeghi, Ghandehariun, & Rosen, 2020b)
11	Asia-southeast	kg H2	-	Cradle-to-gate	-	No	CML	GWP	(Reaño, 2020)
12	North America	kg H2	-	Cradle-to-gate	-	No	CML	GWP & others	(Karaca, Dincer, & Gu, 2020)
13	Europe (Germany)	kg H2	-	Cradle-to-gate	-	Partial (process simulation)	ReCiPe	GWP & others	(Chisalita, Petrescu, & Cormos, 2020)
14	Europe (Central)	MJ H2	-	Cradle-to-gate	-	Partial (process simulation)	ILCD	GWP & others	(Antonini et al., 2020)
15	USA	kg H2	700 bar	Cradle-to-gate	-	No	CML	GWP & others	(Siddiqui & Dincer, 2019)
16	Europe (Netherlands)	GJ H2	-	Cradle-to-gate	-	Partial (process simulation)	Various	GWP & others	(Fernández-Dacosta, Shen, Schakel,

									Ramirez, & Kramer, 2019)
17	Asia (China)	Distance travelled	-	Cradle-to-grave	-	No	CML	GWP & others	(Chen, Hu, & Liu, 2019)
18	-	kg H2	-	Cradle-to-gate	-	Partial (pilot plant)	IMPACT 2002+	GWP & others	(J. Chen et al., 2019)
19	Europe (Germany)	kg H2	-	Cradle-to-gate	-	Partial (laboratory measurements)	ReCiPe	GWP & others	(Bareiß, de la Rua, Möckl, & Hamacher, 2019)
20	-	kg H2	-	Cradle-to-gate	-	No	ReCiPe	GWP & others	(A. Mehmeti, A. Angelis-Dimakis, G. Arampatzis, S. J. McPhail, & S. Ulgiati, 2018)
21	Europe (Denmark)	kg H2	-	Cradle-to-grave	-	No	ILCD	GWP & others	(Zhao & Pedersen, 2018)
22	Europe (Germany)	kg H2	-	Cradle-to-gate	-	No	ILCD	GWP & others	(Wulf & Kaltschmitt, 2018a)
23	Asia (China)	MJ H2	-	Cradle-to-grave	-	No	ReciPe	GWP & others	(Schmidt Rivera, Topriska, Kolokotroni, & Azapagic, 2018)
24	-	kg H2	-	Cradle-to-gate	-	Partial (process simulation)	-	GWP & others	(Salkuyeh et al., 2018)
25	Europe	kg H2	-	Cradle-to-gate	-	Partial (laboratory measurements and calculations)	ReCiPe	GWP & others	(Mehmeti, Angelis-Dimakis, Muñoz, Graziadio, & McPhail, 2018)
26	USA	kg H2	20 bar	Cradle-to-gate	Substitution; (Mass, market value) allocation	No	IPCC	GWP	(Lee, Elgowainy, & Dai, 2018)
27	USA	kg H2	20 bar	Cradle-to-gate	Substitution; (Mass, market value) allocation	No	IPCC	GWP	(Lee & Elgowainy, 2018)
28	Europe (Austria, Germany, Spain)	kg H2	-	Cradle-to-gate	-	No	ReCiPe	GWP & others	(Kuckshinrichs & Koj, 2018)
29	Europe (Austria, Germany, Spain)	kg H2	33 bar, 40 degree C	Cradle-to-gate	-	Partial (pilot project)	ILCD	GWP & others	(J. C. Koj, C. Wulf, A. Schreiber, & P. Zapp, 2017)
30	Canada	kg H2	-	Cradle-to-gate	-	Partial (process simulation)	IPCC	GWP & others	(Khojasteh Salkuyeh, Saville, & MacLean, 2017)
31	Europe (Austria, Germany, Spain)	kg H2	33 bar	Cradle-to-gate	-	No	ILCD	GWP & others	(Hake et al., 2017)
32	-	kg H2	-	Cradle-to-grave	-	No	CML	GWP & others	(Bicer & Dincer, 2017)
33	Canada	kg H2	-	Cradle-to-gate	-	No	CML	GWP & others	(Suleman, Dincer, & Agelin-Chaab, 2016)

34	Canada (Western)	kg H2	60 bar	Cradle-to-gate	-	No	-	GWP	(Ghandehariun & Kumar, 2016)
35	Canada (Western)	kg H2	-	Cradle-to-gate	-	No	-	GWP	(Verma, Olateju, & Kumar, 2015)
36	Canada (Western)	kg H2	-	Cradle-to-gate	-	Partial (measurements, process simulation)	IPCC	GWP	(Verma et al., 2015)
37	Canada	kg H2	-	Cradle-to-grave	-	No	-	GWP	(Cetinkaya, Dincer, & Naterer, 2012)
38	Europe (Italy)	1 MWh of marketable energy products	-	Cradle-to-gate	energy allocation (electricity)	No	CML	GWP & others	(Antonio Valente, Diego Iribarren, Javier Dufour, & Giuseppe Spazzafumo, 2015)
39	USA	ton Methonal (kg H2)	-	Cradle-to-gate	-	No	TRACI	GWP	(D. Ravikumar, Keoleian, & Miller, 2020)
40	Others (Western Australia)	kg H2	80 bar	Cradle-to-gate	-	Partial (mass & energy balance calculation)	-	GWP & others	(Palmer et al., 2021)

9.2 I-BIOREF software platform

Modeling and simulation used for both steam methane reforming (SMR) and alkaline electrolysis (AEC) systems combine comprehensive chemical process analysis in Excel-model basis and in I-BIOREF software platform. The data used for the comprehensive mass, energy and chemical balances analysis originates from the public domain as well as private information provided by biorefinery technology providers.

Chemical process analysis includes an exhaustive list of assumptions (operating conditions, electrochemical coefficients, specific power consumptions, etc.) based on the existing knowledge of the state-of-the-art technologies, complemented by a detailed component-by-component mass balance analysis. In such study, each component inside every stream of the process and their transformation are looked at the same way as in any commercial simulation software in the market. In order to simulate the conversion of materials, stoichiometric, thermodynamic, and kinetic modeling are performed according to the requirement of the models and their level of complexity. Mass balance test, at the end, reassures that each unit operation follows the laws of conservation of mass.

A detailed energy balance study includes the energy demands of each unit operation in terms of fuel, steam, power, effluent treatment, and incorporates the most common integrated structure to accommodate the most energy-optimal configuration as possible. However, thermal optimization of the process is beyond the scope of I-BIOREF and requires the use of other tools such as pinch analysis, which results can later be supplemented to I-BIOREF for further analysis.

Techno-economic analysis is consequently performed by using Capital Expenditures (CAPEX), Operation Expenditures (OPEX), and other pertinent cash flows relevant to the project. CAPEX is estimated according to multiple methods including but not limited to detailed equipment, as well as Total CAPEX. In the detailed equipment approach, the purchase cost of each individual equipment is obtained from accredited sources for a given design parameter which is subsequently used for the scaling of the equipment according to the need of the process. In this approach scaling exponent and installation factor of the equipment, the year index of the reference cost as well as that of the project are all employed to enable a precise calculation of the installed equipment costs. In the Total Capex approach, the user is given the choice to input parameters such as to use a total CAPEX for a reference capacity to calculate the capital costs for the desired capacity. In terms of OPEX, the annual production costs are calculated based on the consumption of chemicals and materials, labor requirements, fixed charges such as taxes and insurance, and other common charges such as plant overhead, distribution, etc. For a complete cash flow study, product revenues together with chemical and material costs are calculated based on the most recent available market prices and costs.

Once the Excel models are tested and validated by multiple biorefinery technology specialists, they are transcribed into CanmetENERGY's .NET platform and implemented into I-BIOREF.

According to Benali et al. in Decision Support Systems for Assessment of Biorefinery Transformation Strategies in The Canadian Journal of Chemical Engineering Journal, I-BIOREF software is an intuitive assessment tool that combines process modelling and simulation, cost evaluation, and environmental impact evaluation to deliver a unique combination of biorefinery technology models and rapidly evaluate trade-offs that reflect the best and most robust biorefinery compromises for the production of bio-based specialty products and commodities.

I–BIOREF is Windows-based and reliable biorefinery evaluation software is possible because the mass and energy balance models in the software have been validated using an established spreadsheet model, such as Excel and Aspen Plus commercial software, while developing the tool with the C#.Net computer-programming language.

I-BIOREF allows modelling of biorefinery processes and simultaneously assessing their technical feasibility, economic viability, and environmental footprint, based on the input and technical performance data collected from Canadian mills and pre-commercial/commercial biorefinery technology providers. I-BIOREF has an automatic control functionality that was incorporated in order to reconcile, diagnose, and communicate inconsistent data or specifications to the user. I-BIOREF computes case-specific performance indicators to assess technical risks when integrating any biorefinery technology model (e.g., yield, purity of the products, incremental demands of resources, productivity, etc.) into existing or new industrial facilities.

I-BIOREF as a flexible software with simulation capabilities is a state-of-the-art decision support tool that creates, models and analyzes industrial biorefinery and bioeconomy projects in a step-wise manner and enables technical, economic, environmental and socio-economic performances of these projects to be quantified. Present and ex-ante scenario analyses driven by changes in controlled technical and economic variables are also some of the benefits of the I-BIOREF designed as a decision support tool.

Further information on the I-BIOREF software platform can be found in the reference (NRCan, 2021).

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