Methodology for Determining the Greenhouse Gas Emissions Associated With the Production of Hydrogen

A Working Paper Prepared by the IPHE Hydrogen Production Analysis Task Force

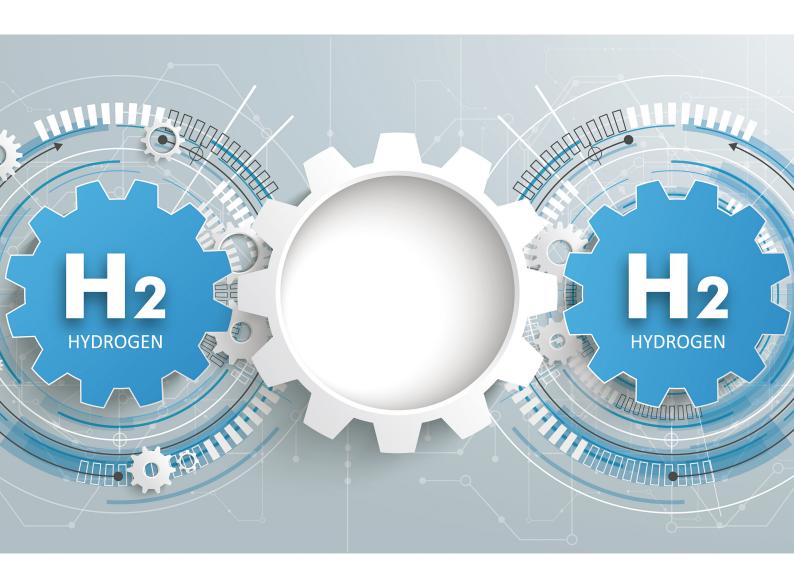


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1 Foreword

Hydrogen can be produced from diverse sources including renewables, nuclear and fossil fuels using carbon capture, utilization, and storage (CCUS) to reduce the emissions associated with its production. Hydrogen can be used to decarbonise numerous sectors including transportation, industrial manufacturing, and power generation. At the Hydrogen Energy Ministerial (HEM) meeting in 2019, Ministers encouraged actions in line with the four pillars in the Tokyo Statement, while taking into account different national circumstances. The versatility and storage capacity of hydrogen creates potential for domestic production and consumption of hydrogen and also as a tradeable energy commodity between countries. There is a need for harmonised regulation, codes, and standards (RCS) to facilitate the deployment of new and innovative technologies. Leading organizations including the International Partnership for Hydrogen and Fuel Cells in the Economy (IPHE), the International Energy Agency (IEA) and Clean Energy Ministerial (CEM) / Mission Innovation (MI) are taking actions on four main issues individually and collaboratively to scale up and accelerate the deployment of hydrogen technologies. This includes collaboration on technologies and harmonization of regulation, codes and standards, and the collection, analysis and sharing of data to evaluate the potential of hydrogen and its effect on CO₂ and other emissions reduction, both upstream and downstream across a variety of hydrogen production pathways.

To enable a robust and sustainable market for hydrogen technologies, it is necessary to develop clean, affordable, secure, and reliable supply chains to support the development of effective hydrogen trading markets. To this end, countries will need to put in place standards and protocols that are transparent and that facilitate efficient international trade in hydrogen. This will require international standards developed through the relevant international standards development bodies, facilitating the removal and/or reduction of regulatory barriers, and to help develop a common definition of clean/sustainable hydrogen.

During the 32nd IPHE Steering Committee in October 2019 in Seoul, South Korea, countries recognised that regulations currently limit the development of a clean hydrogen industry and that government and industry must work together to ensure existing regulations are not an unnecessary barrier to investment. A particular challenge is that identical hydrogen molecules can be produced and combined from sources with very different CO₂ intensities. Likewise hydrogen-based fuels and products be indistinguishable and might result from hydrogen being combined with a range of fossil and low-carbon inputs. Indeed, some of the products made from hydrogen (e.g. electricity) could themselves be used in the production of hydrogen. Accounting standards for different sources of hydrogen along the supply chain will be fundamental to creating a market for low-carbon hydrogen, and that these standards need to be agreed internationally. To this end, a Hydrogen Production Analysis Task Force (H2PA TF) has been created to propose a methodology and analytical framework to determine the GHG emissions related to a unit of produced hydrogen. It may serve as a basis of a certification scheme. However, it will not provide guidance on any GHG emissions intensity threshold values be proposed. This will remain the responsibility of each country even if common terminologies and thresholds will facilitate an international trade of hydrogen.



This methodology is based on the principles of

- inclusiveness (methodologies should not exclude any potential primary energy),
- flexibility (approaches must allow for unique circumstances and hence flexible),
- transparency (methodologies must be transparent in approach and assumptions to build confidence),
- comparability (approach should be comparable with the approach used by other technologies to help allow for 'apples to apples' comparisons on emissions) and
- practicality (methodologies must be practical, facilitating uptake by industry and use in the market).

The emergence of a hydrogen market needs to also increase public knowledge and acceptance. This includes to leverage the increasing demand of information and expectation from the society towards a carbon-neutral economy. In this context, the origin and GHG intensity of hydrogen are important parameters. To facilitate international trade and allow consumers/customers to choose their preferences, there is a need for a (maximum) harmonized international classification framework for hydrogen which includes information on sustainability criteria (e.g. origin, CO₂-intensity, other emissions) across the full lifecycle, usually called from "cradle-to-grave", and which ensures traceability of the attributes. IPHE is open to considering this full lifecycle approach and calls to apply it for all energy vectors. However, based on the previous principles, and in particular to ensure a fair comparability with the other energy vectors, this first version of methodology has adopted the current commonly used system boundaries, usually called from "well-to-gate", excluding the emissions from the building of the capital goods (including hydrogen production devices, etc.). Future IPHE guidance may address additional aspects of the full LCA, such as downstream emissions associated with hydrogen distribution, and emissions associated with manufacturing of goods.

2 Introduction

The H2PA task force aims to initiate a process by taking early steps to develop a mutually agreed upon methodology for determining the greenhouse gas emissions associated with the production of hydrogen. A key issue in the longer term is the certification of CO_2e intensity and origin of hydrogen supplies, as well as benchmarks for the incumbent processes they replace.

A mutually recognised, international framework is needed that is robust, avoids mislabelling or double counting of environmental impacts. The framework will provide a mutually agreed approach to "certificates" of origin, and that covers greenhouse gas inputs to hydrogen-based fuels and feedstock's.

This document presents a methodology that will be built on over time and cover additional production processes where necessary and other parts of the value chain such as different hydrogen physical states and energy carriers, and emissions due to the transportation to the usage gate. It may be this document may be used as a reference by a standard development organisation like ISO (e.g. ISO/TC 197 Hydrogen technologies and ISO/TC 207 Environmental management) to develop an international standard. However, as noted in the H2PA TF terms of reference, this document does not lead to any binding commitments or

expectations on behalf of any country. The methodology serves as a reference with which each county can develop their own methodology by taking into account different national circumstances/regulatory framework.

3 Scope

There are numerous pathways to produce hydrogen from various primary energies. This document describes the requirements and evaluation methods applied to several hydrogen production pathways of interest: electrolysis, steam methane reforming (with carbon capture and storage), by-production and coal gasification (with carbon capture and storage). These are the initial hydrogen production pathways considered by the IPHE H2PA TF. The Taskforce intends to develop analysis methods for other pathways in the future.

This document applies to the evaluation of greenhouse gas emissions in the hydrogen production process in accordance with the life cycle assessment method.

4 Normative References

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 14040 Environmental Management Life Cycle Assessment Principles and Framework

ISO 14044 Environmental Management Life Cycle Assessment Requirements and Guidelines

ISO 14067 Greenhouse gases — Carbon footprint of products — Requirements and guidelines for quantification

GHG Protocol A Corporate Accounting and Reporting Standard. Revised Edition.

5 Terms and Definitions

The common terminology used for the different origins and methods of produced hydrogen investigated in this document is presented in this section. The terms and definitions used by various international organisations (e.g. IEC, ISO) have been adopted whenever possible

5.1 Quantification of the Carbon Footprint of a Product

5.1.1 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]



Note 1: Physical allocation can be applied when a physical, i.e. causal, relationship can be identified between the inputs, outputs and co-products of the multifunctional process. Such a relationship exists when the amounts of the co-products can be independently varied. How the amounts of inputs and outputs (emissions and waste) change following such a variation can be used to allocate the inputs and outputs to the varied co-product

Note 2: This allocation procedure is applicable when: a) the relative production of coproducts can be independently varied through process management, and b) this has causal implications for the inputs required, emissions released or waste produced.

Note 3: inputs and outputs can also be allocated between co-products reflecting other relationships between them, e.g. in proportion to the economic value of co-products (economic allocation). The most common form of economic allocation is based on the revenue obtained from the co-products

[SOURCE: ISO 14040:2006/AMD 1:2020]

5.1.2 Carbon Footprint of a Product, CFP

Sum of greenhouse gas emissions (5.3.5) and greenhouse gas removals in a product system (5.4.3), expressed as CO_2 equivalent (5.3.1) and based on a life cycle assessment (5.5.5) using the single impact category of climate change.

Note 1 to entry: A CFP can be disaggregated into a set of figures identifying specific GHG emissions and removals (see <u>Table 1</u>). A CFP can also be disaggregated into the stages of the life cycle (5.5.4).

Note 2 to entry: The results of the quantification of the CFP are documented in the CFP study report expressed in mass of CO_2e per functional unit (5.3.1).

[SOURCE: ISO 14067:2018]

5.1.3 CFP Study

All activities that are necessary to quantify and report a *carbon footprint of a product* (5.1.2) or a *partial CFP*

[SOURCE: ISO 14067:2018]

5.2 Product Category

Group of products that can fulfil equivalent functions

[SOURCE: ISO 14025:2006, 3.12]

5.2.1 Production Batch

A production batch is the amount of H₂ produced by a registered device between any two points in time selected by the Operator for which the quantity of is calculated



5.2.2 Sub-Batch

A sub batch is the part of a production batch defined in accordance with production process specific calculation procedures

5.2.3 Quantification of CFP

Activities that result in the determination of a carbon footprint of a product (5.1.2) or a partial CFP

Note 1 to entry: Quantification of the CFP or the partial CFP is part of the CFP study

[SOURCE: ISO 14067:2018]

5.3 Greenhouse Gas, GHG

Gaseous constituent of the atmosphere, both natural and anthropogenic, that absorbs and emits radiation at specific wavelengths within the spectrum of infrared radiation emitted by the Earth's surface, the atmosphere and clouds

Note 1 to entry: For a list of greenhouse gases, see the latest IPCC Assessment Report (currently carbon dioxide (CO_2); methane (CH_4); nitrous oxide (N_2O_1)

Note 2 to entry: Water vapour and ozone, which are anthropogenic as well as natural greenhouse gases, are not included in the carbon footprint of a product ()

Note 3 to entry: The focus of this document is limited to long-lived GHGs and it therefore excludes climate effects due to changes in surface reflectivity (albedo) and short-lived radiative forcing agents (e.g. black carbon and aerosols).

[SOURCE: ISO 14067:2018]

5.3.1 Carbon Dioxide Equivalent, CO₂ Equivalent, CO₂e

Unit for comparing the radiative forcing of a greenhouse gas (5.3) to that of carbon dioxide

Note 1 to entry: Mass of a greenhouse gas is converted into CO_2 equivalents by multiplying the mass of the greenhouse gas by the corresponding global warming potential (5.3.4) or global temperature change potential (GTP) of that gas.

Note 2 to entry: In the case of GTP, CO₂ equivalent is the unit for comparing the change in global mean surface temperature caused by a greenhouse gas to the temperature change caused by carbon dioxide.

[SOURCE: ISO 14067:2018]

5.3.2 Emissions

The release of GHG into the atmosphere

[SOURCE: 2004 GHG protocol (Chapter 4)]



5.3.3 Emission Factor

A factor allowing GHG emissions to be estimated from a unit of available activity data (e.g. tonnes of fuel consumed, tonnes of product produced) and absolute GHG emissions

[SOURCE: 2004 GHG protocol (Chapter 6)]

5.3.4 Global Warming Potential, GWP

Index, based on radiative properties of greenhouse gases (GHG) (5.3.5), measuring the radiative forcing following a pulse emission of a unit mass of a given GHG in the present-day atmosphere integrated over a chosen time horizon, relative to that of carbon dioxide (CO_2)

Note 1 to entry: "Index" as used in this document is a "characterization factor" as defined in ISO 14040:2006, 3.37.

Note 2 to entry: A "pulse emission" is an emission at one point in time.

[SOURCE: ISO 14067:2018]

5.3.5 Greenhouse Gas Emission, GHG Emission

Release of a greenhouse gas (5.3.5) into the atmosphere

[SOURCE: ISO 14067:2018]

5.3.6 Greenhouse Gas Emission Factor, GHG Emission Factor

Coefficient relating activity data with the greenhouse gas emission (5.3.5)

[SOURCE: ISO 14067:2018]

5.3.7 GHG Protocol

An additional module of the GHG Protocol Initiative addressing the quantification of GHG Quantification Standard reduction projects. This includes projects that will be used to offset emissions elsewhere and/or generate credits. More information available at: www.GHGprotocol.org

[SOURCE: 2004 GHG protocol (Chapters 8,11)]

5.4 Products, Product Systems and Processes

5.4.1 Product

Any goods or service

NOTE 1 The product can be categorized as follows:

- services (e.g. transport);
- software (e.g. computer program, dictionary);



- hardware (e.g. engine mechanical part);
- processed materials (e.g. lubricant).

NOTE 2 Services have tangible and intangible elements. Provision of a service can involve, for example, the following:

- an activity performed on a customer-supplied tangible product (e.g. automobile to be repaired);
- an activity performed on a customer-supplied intangible product (e.g. the income statement needed to prepare a tax return);
- the delivery of an intangible product (e.g. the delivery of information in the context of knowledge transmission);
- the creation of ambience for the customer (e.g. in hotels and restaurants).

Software consists of information and is generally intangible and can be in the form of approaches, transactions or procedures.

Hardware is generally tangible and its amount is a countable characteristic. Processed materials are generally tangible and their amount is a continuous characteristic.

NOTE 3 Adapted from ISO 14021:1999 and ISO 9000:2005.

[SOURCE: ISO 14040:2006]

5.4.2 Product Flow

Products entering from or leaving to another product system

[SOURCE: ISO 14040:2006]

5.4.3 Product System

Collection of *unit processes* with *elementary flows* and product flows, performing one or more defined functions and which models the *life cycle* (5.5.4) of a *product*

[SOURCE: ISO 14044:2006, 3.28]

5.4.4 Co-Product

Two or more products coming from the same unit process or product system (5.4.3)

[SOURCE: ISO 14040:2006, 3.10]

5.4.5 Energy from Renewable Sources or Renewable Energy

Means energy from renewable non-fossil sources, namely wind, solar (solar thermal and solar photovoltaic) and geothermal energy, ambient energy, tide, wave and other ocean energy, hydropower, biomass, landfill gas, sewage treatment plant gas, and biogas;"

[SOURCE: DIRECTIVE (EU) 2018/2001]



5.4.6 Geothermal Energy

Means energy stored in the form of heat beneath the surface of solid earth

[SOURCE: DIRECTIVE (EU) 2018/2001]

5.4.7 Heating Value

The amount of energy released when a fuel is burned completely. Care must be taken not to confuse higher heating values (HHVs), used in the US and Canada, and lower heating values, used in other countries (for further details refer to the calculation tool for stationary combustion available at www.GHGprotocol.org).

[SOURCE: 2004 GHG protocol]

5.4.8 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]

5.4.9 Intermediate Flow

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

[SOURCE: ISO 14040:2006]

5.4.10 Intermediate Product

Output from a unit process that is input to other unit processes that require further transformation within the system

[SOURCE: ISO 14040:2006]

5.4.11 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]

5.4.12 System Boundary

Boundary based on a set of criteria representing which *unit processes* are a part of the system under study

[SOURCE: ISO 14040:2006/AMD 1:2020]



5.4.13 System Expansion

The concept of expanding the product system to include additional functions related to the co-products can also be referred to as system expansion or expanding the system boundary

Note 1: the product system that is substituted by the co-product is integrated in the product system under study. In practice, the co-products are compared to other substitutable products, and the environmental burdens associated with the substituted product(s) are subtracted from the product system under study. The identification of this substituted system is done in the same way as the identification of the upstream system for intermediate product inputs. See also ISO/TR 14049:2012, 6.4

Note 2: The application of system expansion involves an understanding of the market for the co-products. Decisions about system expansion can be improved through understanding the way co-products compete with other products, as well as the effects of any product substitution upon production practices in the industries impacted by the co-products.

[SOURCE: ISO 14040:2006/AMD 1:2020]

5.4.14 Process

Set of interrelated or interacting activities that transforms inputs into outputs

[SOURCE: ISO 14044:2006]

5.4.15 Functional Unit

Quantified performance of a product system (5.4.3) for use as a reference unit

Note 1 to entry: As the carbon footprint of a product treats information on a product basis, an additional calculation based on a declared unit can be presented (see also 6.3.3).

[SOURCE: ISO 14040:2006, 3.20]

5.4.16 Reference Flow

Measure of the inputs to or outputs from *processes* in a given *product system*) required to fulfil the function expressed by the functional unit

Note 1 to entry: For an example of applying the concept of a reference flow, see the example in <u>6.3.3</u>.

Note 2 to entry: In the case of a partial CFP, the reference flow refers to the declared unit.

[SOURCE: ISO 14067:2018]

5.4.17 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



Note 1 to entry: "Environment" is defined in ISO 14001:2015, 3.2.1.

[SOURCE: ISO 14044:2006]

5.4.18 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]

5.4.19 Functional Unit

Quantified performance of a product system for use as a reference unit

[SOURCE: ISO 14040:2006]

5.5 Life Cycle Assessment

5.5.1 Cut-Off Criteria

Specification of the amount of material or energy flow or the level of significance of greenhouse gas emissions (5.3.5) associated with unit processes or the product system (5.4.3) to be excluded from a CFP study (5.1.3)

Note 1 to entry: "Energy flow" is defined in ISO 14040:2006, 3.13.

[SOURCE: ISO 14067:2018]

5.5.2 Evaluation

Element within the life cycle interpretation phase intended to establish confidence in the results of the life cycle assessment

NOTE Evaluation includes completeness check, sensitivity check, consistency check, and any other validation that may be required according to the goal and scope definition of the study

[SOURCE: ISO 14040:2006]

5.5.3 Fugitive Emissions

Emissions that are not physically controlled but result from the intentional or unintentional releases of GHGs. They commonly arise from the production, processing transmission storage and use of fuels and other chemicals, often through joints, seals, packing, gaskets, etc.

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



5.5.4 Life Cycle

Consecutive and interlinked stages related to a *product* (5.4.1), from raw material acquisition or generation from natural resources to end-of-life treatment

Note 1 to entry: "Raw material" is defined in ISO 14040:2006, 3.15.

Note 2 to entry: Stages of a life cycle related to a product include raw material acquisition, production, distribution, use and end-of-life treatment.

[SOURCE: ISO 14067:2018]

5.5.5 Life Cycle Assessment, LCA

Compilation and evaluation of the inputs, outputs and the potential environmental impacts of a *product system* (5.4.3) throughout its *life cycle* (5.5.4)

Note 1 to entry: "Environmental impact" is defined in ISO 14001:2015, 3.2.4.

[SOURCE: ISO 14044:2006, 3.2]

5.5.6 Life Cycle Inventory Analysis, LCI

Phase of *life cycle assessment* (5.5.5) involving the compilation and quantification of inputs and outputs for a *product* (5.4.1) throughout its *life cycle* (5.5.4)

[SOURCE: ISO 14044:2006, 3.3]

5.5.7 Location-Based Method

Uses the average emissions intensity of the electricity grid in the location in which energy consumption occurs.

[SOURCE: 2015 GHG protocol Scope 2 Guidance]

5.5.8 Market-Based Method

Uses the emissions intensity from choices a consumer makes regarding its electricity supplier or product. These choices (purchasing renewable energy certificates or differentiated electricity product) are reflected through contractual arrangements between the purchaser and the provider.

[SOURCE: 2015 GHG protocol Scope 2 Guidance]

5.5.9 Inventory

A quantified list of an organization's GHG emissions and sources.

[SOURCE: 2004 GHG protocol]

5.5.10 Leakage (Secondary Effect)

Leakage occurs when a project changes the availability or quantity of a product or service that results in changes in GHG emissions elsewhere

[SOURCE: 2004 GHG protocol (Chapter 8)]

5.5.11 Materiality Threshold

A concept employed in the process of verification. It is often used to determine whether an error or omission is a material discrepancy or not. It should not be viewed as a de minimus for defining a complete inventory

[SOURCE: 2004 GHG protocol (Chapter 10)]

5.5.12 Process Emissions

Emissions generated from manufacturing processes, such as the CO₂ that is arises from the breakdown of calcium carbonate (CaCO₃) during cement manufacture. (Chapter 4, Appendix D)

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

5.5.13 Releases

Emissions to air and discharges to water and soil

[SOURCE: ISO 14040:2006]

5.5.14 Scope

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

[SOURCE: 2004 GHG protocol (Chapter 4)]

5.5.15 Scope 1 Inventory

A reporting organization's direct GHG emissions

[SOURCE: 2004 GHG protocol (Chapter 4)]

5.5.16 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)]

5.5.17 Scope 3 Inventory

A reporting organization's indirect emissions other than those covered in scope 2

[SOURCE: 2004 GHG protocol (Chapter 4)]



5.5.18 Sensitivity Analysis

Systematic procedures for estimating the effects of the choices made regarding methods and data on the outcome of a *CFP study* (5.1.3)

[SOURCE: ISO/FDIS 14067:2018]

5.5.19 Sensitivity Check

Process to determine whether the information obtained from a sensitivity analysis is relevant for reaching the conclusions and for giving recommendations

[SOURCE: ISO 14040:2006 FDAM 1:2020]

5.5.20 Transparency

Open, comprehensive and understandable presentation of information

[SOURCE: ISO 14040:2006]

5.5.21 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]

5.5.22 Waste

Substances or objects that the holder intends or is required to dispose of

Note 1 to entry: This definition is taken from the Basel Convention on the Control of Transboundary Movements of Hazardous Wastes and Their Disposal (22 March 1989), but is not confined in this document to hazardous waste.

[SOURCE: ISO 14040:2006, 3.35]

5.6 Organizations

5.6.1 Interested Party

Individual or group concerned with or affected by the environmental performance of a product system, or by the results of the life cycle assessment

[SOURCE: ISO 14040:2006]

5.6.2 Intergovernmental Panel on Climate Change (IPCC)

The Intergovernmental Panel on Climate Change (IPCC) is the international body for assessing the science related to climate change. The IPCC was set up in 1988 by the World



Meteorological organization (WMO) and United Nations Environment Programme (UNEP) to provide policymakers with regular assessments of the scientific basis of climate change, its impacts and future risks, and options for adaptation and mitigation. (www.ipcc.ch).

[SOURCE: IPCC factsheet]

5.6.3 Organization

Person or group of people that has its own functions with responsibilities, authorities and relationships to achieve its objectives

Note 1 to entry: The concept of organization includes, but is not limited to, sole-trader, company, corporation, firm, enterprise, authority, partnership, charity or institution, or part or combination thereof, whether incorporated or not, public or private.

[SOURCE: ISO 14001:2015, 4]

5.7 Data and Data Quality

5.7.1 Data Quality

Characteristics of data that relate to their ability to satisfy stated requirements

[SOURCE: ISO 14040:2006]

5.7.2 Double Counting

Two or more reporting companies take ownership of the same emissions or reductions

[SOURCE: 2004 GHG protocol (Chapters 3, 4, 8, 11)]

5.7.3 Primary Data

Quantified value of a *process* (5.4.14) or an activity obtained from a direct measurement or a calculation based on direct measurements

Note 1 to entry: 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 to entry: Primary data can include greenhouse gas emission factors and/or greenhouse gas activity data (defined in ISO 14064-1:2006, 2.11).

[SOURCE: ISO 14067:2018]

5.7.4 Secondary Data

Data which do not fulfil the requirements for primary data (5.7.3)

Note 1 to entry: 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 to entry: Secondary data can include data obtained from proxy processes or estimates.

[SOURCE: ISO 14067:2018]

5.7.5 Site-Specific Data

Primary data obtained within the product system

Note 1 to entry: 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 to entry: 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]

5.7.6 Uncertainty

Parameter associated with the result of quantification that characterizes the dispersion of the values that could be reasonably attributed to the quantified amount

Note 1 to entry: Uncertainty can include, for example:

- parameter uncertainty, e.g. greenhouse gas emission factors, activity data;
- scenario uncertainty, e.g. use stage scenario, end-of-life stage scenario;
- model uncertainty.

Note 2 to entry: Uncertainty information typically specifies quantitative estimates of the likely dispersion of values and a qualitative description of the likely causes of the dispersion.

[SOURCE: ISO 14067:2018]

5.8 Abbreviated Terms

CCS CO₂ Capture and Storage
CCU CO₂ Capture and Utilisation
CFP Carbon Footprint of a Product
CO₂e Carbon Dioxide Equivalent

GHG Greenhouse Gas

GWP Global Warming Potential

IPCC Intergovernmental Panel On Climate Change

LCA Life Cycle Assessment



LCIA Life Cycle Impact Assessment
LCI Life Cycle Inventory Analysis

LHV Low Heating Value

MDEA Mono-Diethanol Amine
MEA Mono-Ethanol Amine

NG Natural Gas

PSA Pressure Swing Adsorption
SMR Steam Methane Reformer

6 Evaluation Methods

6.1 Evaluation Basis

The proposed emissions accounting methodology aims at being applied for all hydrogen production pathways utilising the different standards ISO 14067, ISO 14040, ISO 14044 and the GHG protocols that represent a universally recognized methodology to study the carbon footprint (and other impacts) of fuel production.

Therefore, referring to ISO 14067, the following criteria shall be applied for the goal and scope definition phase:

- a. the product category definition and description of the investigated pathways are identical;
- b. the declared unit is identical;
- c. the system boundary is equivalent;
- d. the description of data is equivalent;
- e. the criteria for inclusion of inputs and outputs are equivalent;
- f. the data quality requirements (e.g. coverage, precision, completeness, representativeness, consistency and reproducibility) are the same;
- g. assumptions especially for the delivery stage are the same;
- h. specific GHG emissions and removals are treated identically;
- i. the units (described in Annexes) are identical;

The following criteria shall be applied for the life cycle inventory and LCIA phase:

- j. the methods of data collection and data quality requirements are equivalent;
- k. the calculation procedures are identical;
- I. the allocation of the flows is equivalent;
- m. the applied GWPs are identical.

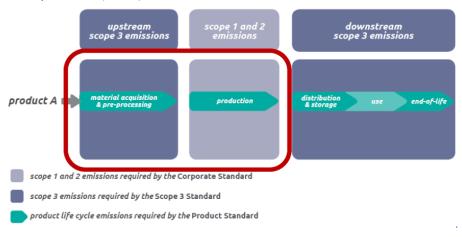
6.2 Evaluation Scope

6.2.1 Product System Boundary

Analysis methods described in the current IPHE guidance cover a "well-to-gate" system boundary, including Scope 1, Scope 2, and partial Scope 3 emissions and excluding emissions



deemed immaterial per Section 6.2.2. Partial Scope 3 emissions considered include associated impacts from the raw material acquisition phase, raw material transportation phase, hydrogen production and manufacture. GHG contributions are defined in terms of carbon dioxide equivalent (CO₂e)



Source: Green House Gas Protocol: Product life Cycle Accounting and Reporting Standard - WBCSD, WRI

Figure 1: "Well-to-Gate" system boundary adopted for this document

The emissions from the construction, manufacturing, and decommissioning of the capital goods (including hydrogen production device, etc.), business travel, employee commuting and upstream leased assets are not considered. The rationale for this simplification was motivated by the comparatively small contribution that these emissions add to emissions associated with both fossil and renewable pathways,¹ and the fact that they are expected to decrease rapidly in the future,^{2,3,4,5} due to effects of technological progress, and concurrent decarbonisation of upstream energy and material production, such as aluminium, clinker, copper or steel.

If buffer storage is integrated with hydrogen production within the plant, then emissions associated energy consumption related to the operation of hydrogen storage facilities within the plant should be included.

⁵ Assessment Report of the Intergovernmental Panel on Climate Change [Edenhofer, O., R. Pichs-Madruga, Y. Sokona, E. Farahani, S. Kadner, K. Seyboth, A. Adler, I. Baum, S. Brunner, P. Eickemeier, B. Kriemann, J. Savolainen, S. Schlömer, C. von Stechow, T. Zwickel and J.C. Minx (eds.)]. Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA



¹ Pehl, M., Arvesen, A., Humpenöder, F., Popp, A., Hertwich, E. G., & Luderer, G. (2017). Understanding future emissions from low-carbon power systems by integration of life-cycle assessment and integrated energy modelling. Nature Energy, 2(12), 939–945. https://doi.org/10.1038/s41560-017-0032-9

² Pehl, M., Arvesen, A., Humpenöder, F., Popp, A., Hertwich, E. G., & Luderer, G. (2017). Understanding future emissions from low-carbon power systems by integration of life-cycle assessment and integrated energy modelling. Nature Energy, 2(12), 939–945. https://doi.org/10.1038/s41560-017-0032-9

³ Hertwich, E. G., Gibon, T., Bouman, E. A., Arvesen, A., Suh, S., Heath, G. A., Shi, L. (2014). Integrated life-cycle assessment of electricity-supply scenarios confirms global environmental benefit of low-carbon technologies. Proceedings of the National Academy of Sciences of the United States of America. https://doi.org/10.1073/pnas.1312753111, 10.1073/pnas.1312753111

⁴ Hydrogen decarbonisation pathways - A life-cycle assessment Hydrogen Council (2021)

As the downstream boundary limit, the point of production of hydrogen (at gate) is considered for the functional unit at a default pressure level greater than or equal to 3 MPa⁶ (classical output pressure form the most used SMR production pathway) and a purity at gate greater or equal to 99 % (an evaluation of GHG emission impact if moving to 99.9% or even 99.95% could be considered). Emissions associated with hydrogen infrastructure past the hydrogen production gate (e.g. liquefaction, hydrogenation in a carrier) and transportation to the consumption location will be considered in separate documents.

There are many process routes for hydrogen production, and different processes and methods are being proposed and implemented. This document gives the evaluation principles, system boundaries and expected reported metrics for four main routes. Appendixes A to D present the system boundaries of typical hydrogen production methods in hydrogen production from electrolysis of water, hydrogen production from steam reforming of natural gas with CCS, hydrogen production from industrial by-products and hydrogen production from coal gasification with CCS.

6.2.2 Selected Cut-Off Criteria

In general, efforts shall be taken to include all processes and flows that are attributable to the analysed system. Completeness based on environmental significance should be tested by including and excluding processes in the system boundary to determine if results change⁷.

If individual material or energy flows are found to be insignificant for a particular unit process, these may be excluded and shall be reported as data exclusions considering that if the actual data is known, then it should be included and not considered for exclusion. The cut-off criteria used to exclude certain processes of minor importance shall be clearly and consistently defined within the goal and scope definition phase.

Cut-off criteria for exclusion from analysis include:

- (1) uncertainty of the measurement equipment;
- (2) if regular and/or on-line measurements are unavailable, use proxy data derived from the open literature and applicable to the H₂ production location;

The final sensitivity analysis of the inputs and outputs data shall include the mass, energy and environmental (expressed in CO_2e/kg_{H2}) significance criteria so that all inputs not considered in the study must be reported.

⁷ Testing for completeness based on environmental relevance is defined by ISO 14044 to be based on three criteria: mass, energy and environmental significance.



⁶ For technologies whose typical hydrogen output pressure at gate is 1 MPa or lower, one can also report GHG emission at 1 MPa in addition to the GHG emission at 3 MPa. Calculation result of GHG emission adjusted to 3 MPa will require additional energy to compress the output pressure to 3 MPa using the same electricity emission factor as in 6.3.3.2.1.

6.2.3 Evaluation Elements

The life cycle assessment of GHG emissions of produced hydrogen selects the impact of climate change as the evaluation element. The characteristic factors are shown in the following Table 1:

Table 1: Types of environmental impacts and characteristic factors

Environmental impact type	Characterization model	Unit
Climate change	Global warming potential (GWP100)	kgCO₂e

Greenhouse gases considered in this study are carbon dioxide (CO₂), methane (CH₄), and nitrous oxide (N₂O)⁸. The global warming potential (GWP) of the various greenhouse gases is expressed in CO₂e.

Table **2** shows the GWP for a period of 100 years according to the Fifth Assessment Reports of the Intergovernmental Panel on Climate Change (IPCC).

Table 2: Global warming potential (GWP) of various GHGs [IPCC 2018]

<u> </u>		
	AR5 CO ₂ e (g/g)	
CO ₂	1	
CH ₄	28	
N ₂ O	265	

Following the product system boundaries, the energy requirements and GHG emissions resulting from the construction and decommissioning of manufacturing plants are not considered here. Furthermore, energy requirements and emissions resulting from the manufacturing and decommissioning of installations or applications (e.g. vehicles) consuming the hydrogen are not considered.

and, GHG impact of electricity used for H_2 production shall be restricted to Scope 1 and 2 emissions, and partial Scope 3 assumptions (not including emissions associated with manufacturing of power generation facilities). As a result, the GHG impact of electricity generation from wind, solar photovoltaic, hydropower and geothermal will be assumed to be zero⁹.

6.2.4 Evaluation Cycle

The hydrogen considered should be evaluated with hydrogen produced in an industrial plant as the object.

The evaluation cycle for data is the considered time period of hydrogen production for which the quantified figure for the GHG emissions are representative. The time period for which the GHG emissions are representative shall be specified and justified.

⁹ There are some countries as e.g. Japan, whose electricity from wind, solar photovoltaic, hydropower and geothermal represent avoided emissions compared with average national grid emissions. In these cases, GHG impacts are not considered as zero so that the residual mix concept is not applicable.



 $^{^{8}}$ Other greenhouse gases are e.g. CFCs, HFCs, and SF $_{6}$, which are, however, not relevant in this context

All GHG emissions and removals shall be calculated, at least yearly, as if released or removed at the beginning of the assessment period without taking into account an effect of delayed GHG emissions and removals.

The choice of the time period for data collection should consider intra- and inter-annual variability and, when possible, use values representing the trend over the selected period. Where the GHG emissions and removals associated with specific unit processes within the life cycle of a product vary over time, data shall be collected over a time period appropriate to establish the average GHG emissions and removals associated with the life cycle of the product.

6.3 Life Cycle Impact Assessment

The process, methods and requirements of hydrogen life cycle impact assessment refer to ISO 14044.

A description of the following items is given for the hydrogen production pathway.

- Hydrogen production process overview and description
- emissions accounting method
- emissions inventory
- energy supply
- embodied emissions relating to the upstream extraction of resources
- emissions allocation
- results of sensitivity analyses and uncertainty assessments
- results of the life cycle interpretation, including conclusions and limitations
- disclosure and justification of value choices that have been made in the context of decisions within the study
- description of the stages of the life cycle, including a description of the selected use profiles when applicable
- assessment of influence of alternative use profiles on the final results
- time period for which the partial carbon footprint is representative
- reference used in the study.

6.3.1 Description of Data

The methodology should use data that reduces bias and uncertainty by using the best quality data available. Data quality shall be characterized by both quantitative and qualitative aspects.

Characterization should address the following:

- a. time-related coverage: age of data and the minimum length of time over which data should be collected;
- b. geographical coverage: geographical area from which data for unit processes should be collected to satisfy the goal of the partial carbon footprint study;
- c. technology coverage: specific technology or technology mix;
- d. precision: measure of the variability of each data value expressed (e.g. variance);
- e. completeness: percentage of total flow that is measured or estimated;



- f. representativeness: qualitative assessment of the degree to which the data set reflects the true population of interest (i.e. geographical coverage, time period and technology coverage);
- g. consistency: qualitative assessment of whether or not the study methodology is applied uniformly to the various components of the sensitivity analysis;
- h. reproducibility: qualitative assessment of the extent to which information about the methodology and data values would allow an independent practitioner to reproduce the results reported in the partial carbon footprint study;
- i. sources of the data;
- j. uncertainty of the information.

6.3.2 Emissions Accounting

An overview of the GHG emissions accounting methodology applied to each production pathways is summarised below.

Emissions include all Scope 1 and 2 and partial Scope 3 emissions¹⁰ arising in the "well-to-gate" boundary as defined in section 6.2.1.Carbon capture storage removals are defined in accordance with IPCC guidelines (not applicable for electrolysis).

Emissions of co-products are either discretely measured or accounted for through another means (see Section 6.3.3.4). CO₂ is not to be considered as a co-product.

The final accounted emissions will be the total emissions subtracted by the CCS removals and the emissions accounted to the co-products.

6.3.3 Emissions Inventory

The equation below shows the breakdown of the emissions inventory into its components (emissions categories). Individual countries may use their own emissions inventory that aligns with IPCC guidelines.

 $E_{emissions}$ inventory = $E_{combustion}$ emissions + $E_{fugitive}$ emissions + $E_{industrial}$ process emissions + E_{emergy} supply emissions + $E_{embodied}$ emissions

6.3.3.1 Combustion Emissions

This source refers to the combustion of relevant solid, liquid and/or gaseous fuels including (but not limited to) coal, diesel and natural gas. Combustion emissions can be estimated via a variety of approaches including use of emission factors and measurement of fuel (volumetric or gravimetric), and direct measurement.

Combustion emissions should be calculated as follows:

$$E_{\text{combustion}} = \sum_{i} E_{\text{combustion,i}}$$

Where E_{combustion} is the sum of emissions of carbon dioxide, methane and nitrous oxide (as applicable), released from the combustion of fuel type (i) within the module measured and



converted in CO₂e. This covers combustion of solid, liquid, and gaseous fuels calculated using a variety of methods.

6.3.3.2 Fugitive Emissions

This source intends all structural and operational losses due to the technology deployed and plant management respectively. Therefore, leakages and accidental losses, as well as other losses due to not-correct managing plant operations, are considered fugitive emissions. Fugitive emissions should be calculated as follows:

$$E_{\text{fugitive}} = \sum_{i} E_{\text{fugitive,i}}$$

Where $E_{fugitive}$ is the sum of structural and operational emissions of carbon dioxide, methane and nitrous oxide (as applicable), released from fugitives of source type (i) within the module measured in CO_2e .

For coal mining, this includes underground and open cut mines and emissions from coal extraction and flaring of coal mine waste gas. However, consistent with the well-to-gate system boundary, activities associated with the decommissioning of the facility (fugitives associated with post-mining activities) should be excluded.

As for most hydrogen producers, fossil fuels are provided by a third party, fugitive emissions associated to its transmission and distribution are captured by embodied emissions.

6.3.3.3 Industrial Process Emissions

Refers to emissions of specific GHG gases used across a number of industry activities (e.g. hydrofluorocarbons (HFCs) used in industrial refrigeration and/or cooling systems, and sulphur hexafluoride (SF6) used in electrical switchgear). For the purposes of this methodology, this is expected to be limited to emissions of CH_4 and N_2O .

There are a variety of approaches that may be employed to estimate these emissions. Typically this might be via assumed leakage rates, or changes in stock levels of the relevant substances as measured throughout the relevant batch period. These items are expected to be extremely minor sources, and estimation should be sufficient in most cases. Industrial process emissions should be calculated as follows:

$$E_{\text{industrial process emisisons}} = \sum_{i} E_{\text{industrial process emisisons,i}}$$

Where $E_{industrial}$ process emissions is the sum of emissions of relevant GHG (as applicable), released from industrial process activity (i) within the module measured in CO_2e tonnes.

6.3.3.4 Energy Supply

For the location-based emissions accounting approach, energy supply emissions should be calculated as follows:

$$E_{\text{energy supply emissions,location}} = \sum_{i} E_{\text{energy supply emissions,i}}$$

Where Eenergy supply emissions, location is the emissions of carbon dioxide, methane and nitrous oxide (as applicable), associated with supply of energy (i) within the module measured in CO_2e tonnes (calculated in line with the location-based approach). For the market-based emissions accounting approach, net energy supply emissions should be calculated as follows:



 $E_{\text{net energy supply emissions,market}} = \sum_{i} E_{\text{energy supply emissions,i}} - E_{\text{applicable renewable energy}}$

Where:

- E_{energy supply emissions,market} is the emissions of carbon dioxide, methane and nitrous oxide (as applicable), associated with supply of energy (i) within the module measured in CO₂e tonnes (calculated in line with the market-based electricity approach);
- E_{applicable renewable energy} is the emissions associated with the supply of energy (in MWh) for which relevant renewable energy certificates have been purchased and retired.

6.3.3.4.1 Treatment of Electricity

The GHG emissions associated with the use of electricity shall include:

- GHG emissions arising from the life cycle of the electricity supply system, such as
 upstream emissions (e.g. the mining and transport of fuel to the electricity generator
 or the growing and processing of biomass for use as a fuel). Emissions associated
 with capital equipment manufacturing, construction and decommissioning are
 excluded;
- GHG emissions during generation of electricity, including losses from electricity generation process and from transmission and distribution.

a) On-site electricity generation (scope 1 emissions)

When electricity is internally generated (e.g. on-site generated electricity) and consumed for the investigated hydrogen production process and no contractual instruments have been sold to a third party, then the emissions would be any scope 1 emissions resulting from generating that electricity.

Following the product system boundaries, Scope 1 emissions from electricity use are considered to be zero if on-site renewable electricity is used.

b) Electricity from the grid (scope 2 emissions)

A GHG emission factor obtained from the organization's supplier for the consumed electricity may be used if there is a dedicated transmission line between the organization and the generation plant from which the GHG emission factor is derived, and no contractual instruments have been sold to a third party for that consumed electricity.

The GHG electricity emissions should refer to electricity consumed by the plant, considering upstream emissions, operational and downstream emissions and all losses in electricity generation facility and transmission and distribution losses.

The electricity emissions reporting method proposed is consistent with the GHG protocolⁱ. This approach includes dual reporting requirements consisting of a location-based and market-based method.

• The location-based method to depict emissions with reference to the average emissions from the relevant regional grid at the time of the production measured in hours¹¹;

¹¹ Location-based method – uses the average emissions intensity of the electricity grid in the location in which energy consumption



- The market-based method to depict a businesses' emissions with reference to its renewable energy investments, such as power purchase agreements (PPA) or purchase of renewable energy certificates. This approach enables businesses to reduce their scope 2 emissions through contractual arrangements for renewable energy;
- Market-based data will be used where possible to calculate emissions-intensity of hydrogen production;
- If a market-based method is used, and the structure of regional regulations or renewable energy markets create potential for double counting of renewable energy between the market-based and location-based approaches, then a *residual mix* factor should be applied to the residual electricity that is not covered by contractual arrangements¹²;
- the residual mix factor may be country specific or average location-based grid emissions;
- all contractual instruments used in the market-based method must meet the scope 2 quality criteria listed in the GHG Protocol Scope 2 Guidance (Table 7.1, page 60).

A **residual mix factor** is applied to depict the emissions intensity of electricity consumed that is not covered by contractual arrangements. This factor will vary by country and potentially within regions of the same country, depending on how contracts for renewable energy are implemented. If the renewable energy a hydrogen producer consumes via contractual arrangements (e.g. renewable electricity credits or PPA) is not represented in the regional grid emissions factor, then the residual mix factor can just represent the emissions factor of the grid. If, however, renewable energy being consumed by contracts is represented in the regional grid factor, then the residual mix factor must mitigate double counting. The manner in which this factor is calculated will vary based on the region and its associated regulations.

Consumers who do not make specified purchases should use the residual mix factor to calculate their market-based total.

In case of electricity import, a distinction between renewable and non-renewable electricity may be made. For the non-renewable electricity, the emission factor from the export country has to be used.

For the location-based approach, the quantity of electricity consumed is multiplied by the average grid emission factor, in kilograms of CO₂e emissions per kilowatt hour, for the region in which the consumption occurs. State or province level grid factors are preferred but country level grid factors may also be applied if State or province factors are not available.

¹² Double counting could occur if the same unit of renewable energy is sold to a hydrogen producer via contractual arrangements (e.g. renewable energy credits) and also accounted for in the renewable content of the regional grid. To mitigate double counting in such situations, if a hydrogen producer is using the market-based method, a residual mix factor should be used to depict the emissions intensity of the regional grid.



6.3.3.5 Steam Supply

For steam supply (i.e. where steam is purchased from some third party provider) emissions should be accounted for by the supplier with an emission factor provided to the buyer for use. These need to be well documented with complete data on fuel used, efficiency of conversion and all losses or leakages.

6.3.3.6 Embodied Emissions

Embodied emissions (other than the energy supply emissions covered above) refers to upstream emissions associated with any input to a system. This could include key inputs such as coal, oxygen and natural gas. Additional input streams may be considered on an as needed basis, pending materiality. This could include items such as salts used for electrolysis and chemicals used for water treatment.

All processing associated with system water supply is assumed to occur within the facility boundaries and thus all emissions associated with this stream should be captured¹³.

Where multiple modules are considered, the emissions associated with the output or intermediate product of this module are associated with embodied emissions which should be carried into subsequent module(s).

The overall calculation for estimation of embodied emissions is as follows:

$$E_{\text{embodied emissions}} = \sum_{i} E_{\text{embodied emissions,i}}$$

Where E_{embodied emissions} is the emissions of carbon dioxide, methane and nitrous oxide (as applicable), associated with input (i) within the module measured in CO2e tonnes.

6.3.3.7 Emissions Allocation

Production pathways for hydrogen always result in various waste products, by-products and co-products.

ISO 14044 and the GHG Protocol Standard distinguish between the product which is being studied as part of the GHG inventory preparation and other co-product(s) which "have value as an input into another product's life cycle" (GHG Protocol, 2011). Consequently, the total emissions resulting from the hydrogen production should be separated between the hydrogen and the number of co-products where these products are valorised (on-sold). This **allocation** refers to the partitioning of the inputs or outputs of a process or product system between the product system under study and one or more other product systems. Waste products have no emissions allocated and by-products are assumed as co-products in terms of GHGs allocation criteria.

¹³ Where water supply has been treated/processed upstream emissions for this supply should be considered in building the emissions inventory.



ISO 14044 states that allocation may be avoided by expanding the product system to include the additional functions related to the co-products. ISO 14044;2006/AMD 2:2020, Annex D document describes allocation procedures. There is no priority given between system expansion and physical allocation. The strengths and weaknesses of each one is described. There are some risks with the system expansion approach if not properly defined and implemented which could lead to some unintended consequences. For instance, in case of electricity as co-product, the use of system expansion approach can result in a broad range of values for the emissions-intensity attributed to hydrogen, based on the emission intensity of the local grid (which may vary significantly between regions and countries).

Where 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. As discussed in section 6.3.3.4.1, physical allocation could be performed on a mass basis or energy content basis. Energy is the most applicable to hydrogen production due to its high energy to mass ratio.

The methods for each production pathway will include specific guidance on the allocation approach to be used for each product. Allocation procedures shall be uniformly applied to similar inputs and outputs of the product system under consideration. The sum of the allocated inputs and outputs of a unit process shall be equal to the inputs and outputs of the unit process before allocation.

The procedures to manage coproducts for the shared unit processes should use the following order if feasible:

- Allocation based on Energy content (physical allocation);
- Allocation based on System expansion;
- Allocation based on Economic value.

6.3.3.7.1 Energy Content (Physical Allocation)

Physical allocation can be applied when a physical, i.e. causal, relationship can be identified between the inputs, outputs and co-products of the multifunctional process. Such a relationship exists when the amounts of the co-products can be independently varied. How the amounts of inputs and outputs (emissions and waste) change following such a variation can be used to allocate the inputs and outputs to the varied co-product.

This allocation procedure (step 2, 4.3.4.2 of ISO 14044) is applicable when:

- a) the relative production of co-products can be independently varied through process management, and
- b) this has causal implications for the inputs required, emissions released or waste produced.

Physical allocation is based on physical constants, resulting in allocation, meaning the allocation factors that are relatively stable. But in many cases, physical allocation needs a deep insight into the process shared with other product systems. For co-products with significantly different economic values, physical allocation will not always properly reflect



the intention to operate the process. Sometimes results based on physical allocations lead to interpretations that are disconnected from the business reality. When there is limited capacity to independently vary the production of co-products, the physical allocation procedure can have limitations. Allocation on a mass basis is problematic for hydrogen production as hydrogen has a high energy to mass ratio compared to the other co-products. This approach is therefore not recommended as a priority.

Allocation on the basis of energy content (the amount of useful energy contained in each co-product) could be suitable in many instances as hydrogen is an energy product. However not all co-products contain useful energy (such as oxygen, chlorine) and in this case energy content would not be a meaningful basis for allocation and another method could be used.

6.3.3.7.2 System Expansion with Displacement

Expanding the product system to include additional functions related to the co-products (see 4.3.4.2, step 1, option 2 of ISO 14044) can be a means of avoiding allocation.

In the system expansion method, co-products are considered alternatives to other products on the market and can be assigned the same environmental burden as the alternative product. Therefore, the alternative product system that is substituted for the co-product is integrated in the product system under study. In practice, the co-products are compared to other substitutable products, and the environmental burdens associated with the substituted product(s) are subtracted from the product system under study (see Figure 2). The identification of this substituted system is done in the same way as the identification of the upstream system for intermediate product inputs.

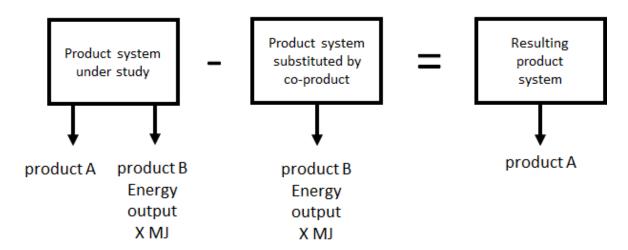


Figure 2: Example of avoiding allocation by expanding the system boundary 14

The application of system expansion involves an understanding of the market for the coproducts. Decisions about system expansion can be improved through understanding the

¹⁴ ISO 14044:2006 / FDAM 2:2020¹⁵ ISO/TS 14071 Environmental management — Life cycle assessment — Critical review processes and reviewer competencies: Additional requirements and guidelines to ISO 14044:2006



way co-products compete with other products, as well as the effects of any product substitution upon production practices in the industries impacted by the co-products.

Important considerations relating to the identification of product systems substituted by coproducts include whether:

- specific markets and technologies are affected;
- the production volume of the studied product systems fluctuates in time;
- a specific unit process is affected directly.

If applicable, when the inputs are delivered through a market, it is also important to know:

- whether any of the processes or technologies supplying the market are constrained, in which case their output does not change in spite of changes in demand;
- which of the unconstrained suppliers/technologies has the highest or lowest production costs and, therefore, is the supplier/technology affected when the demand for the supplementary product is generally decreasing or increasing, respectively.

The justification of the choice of system expansion can be based on technical considerations. System expansion can often be a straightforward choice for energy products. But where there are multiple industrial pathways for co-products, the model results can have high variability. If there are different possibilities of system expansion, it can lead to significantly different results. It is not always straightforward to identify. Therefore, the substitute systems for each co-product where system expansion is used have been precisely defined. This will ensure that, for a particular co-product, all hydrogen producers use the same substitute system.

It is not always straightforward to identify the products that are assumed to be substituted by the co-products of the multifunctional process. If there are no alternative production processes for a co- product, then system expansion is difficult to treat the multifunctional process and another means of allocation has been identified.

6.3.3.7.3 Economic Value

According to 4.3.4.2, step 3 of ISO 14044, inputs and outputs can also be allocated between co-products reflecting other relationships between them, e.g. in proportion to the economic value of co-products (economic allocation).

The most common form of economic allocation is based on the revenue obtained from the co-products.

Economic allocation can reflect the intention of operating a process. The relative revenues can in some situations be seen as the ultimate causes for the production to take place. Economic allocation can help to reflect differences between regions and markets for similar products. Economic allocation has the potential to differentiate between similar products having different quality attributes. But market prices often vary with time, and between different regions and market actors. The selection of the allocation factors represents a value choice and the allocation factor can show a high uncertainty, especially for future



scenarios. The application of economic allocation depends on having market prices for all co-products at the process of co-production. In general, a cost- or revenue-allocated product system will therefore not reflect the physical causalities of producing or purchasing a specific product. Therefore, economic allocation is only used when energy allocation or system expansion cannot be applied.

6.4 Life Cycle Assessment Report

After completing the life cycle impact assessment, the applicant should prepare a life cycle assessment report. The content of the report refers to ISO 14044.

7 Evaluation Process

7.1 Application

The applicant shall submit a formal verification application to the public service platform recognized by the national energy authority.

7.2 Document Verification

The public service platform may entrust a third-party verification agency to review the documents provided by the applicant unit in accordance with the requirements of this document¹⁵.

7.3 On-Site Verification

After completing the document verification, the verification agency shall conduct on-site verification based on this document and the documents submitted by the applicant. The on-site verification period is up to the verification agency but has to take place at least after any changes in the process or feedstock.

7.3.1 Document Verification and Submission Materials

- a) A scanned copy of the application unit's business license;
- b) The hydrogen production flow chart of the application unit;
- c) The main equipment list for hydrogen production;
- d) The life cycle of hydrogen production Evaluation report;
- e) List of raw materials for hydrogen production and their associated GHGs emissions;
- f) Energy/mass flow diagram;
- g) Energy metering system diagram;
- h) If hydrogen production facilities and equipment involve multiple locations, a list of production locations, processes, and processes of each facility should be submitted. Production date and production capacity information;
- i) Where other units apply for hydrogen evaluation for hydrogen production units, the relationship between the parties and the use of hydrogen evaluation shall be explained.

 $^{^{15}}$ ISO/TS 14071 Environmental management — Life cycle assessment — Critical review processes and reviewer competencies: Additional requirements and guidelines to ISO 14044:2006



7.4 On-Site Verification Steps

- a) Site visits and surveys;
- b) Confirm the input and output information of the product system boundary and unit process;
- c) Confirm the completeness and standardization of the data collection plan and data collection process;
- d) Check on-site data and time. The accuracy of the level data and the consistency of the data source;
- e) Check whether the content of the hydrogen life cycle assessment report meets the requirements of this document, and whether the information is correct;
- f) On-site verification of hydrogen parameters produced by hydrogen production projects, such as hydrogen purity, hydrogen pressure, hydrogen production, etc. Hydrogen production projects should have equipment to measure these hydrogen parameters and have a calibration certificate within the validity period.

8 Evaluation Conclusion

After completing the document verification and on-site verification in accordance with the requirements of this standard, the verification agency shall issue the evaluation conclusion.

Appendix A Hydrogen Production Pathway - Electrolysis

There are currently three main electrolyser technologies, distinguished by the electrolyte (and associated production temperatures): alkaline electrolyser, polymer electrolyte membrane (PEM) electrolyser and solid oxide (SOEC) electrolyser. This methodology may be applied to any other electrolysis technologies.

A.1 Electrolysis Process Description

A water electrolysis cell consists of an anode and a cathode separated by a membrane immerged in an electrolyte (a conductive solution). When connected to a direct current power supply, electricity flows through the electrolyte and causes the water to split into hydrogen and oxygen. Each electrolyser system consists of a stack of electrolysis units, a gas purifier and dryer and an apparatus for heat removal.

Hydrogen and oxygen gas products must be purified, dried and cooled prior to storage and/or delivery to market, subject to required product specifications.

The oxygen gas must be safely vented to the atmosphere. Alternatively, pending availability of appropriate markets, this oxygen may be sold as a co-product.

Within this emissions accounting framework, electrolyzers are assumed to have an outlet pressure of 3 MPa¹⁶. Depending on the design of the electrolyzer, an electrolysis system may require compression to achieve 3 MPa pressure or drying. In that case, energy consumption for achieving this and the associated emission have to be calculated and included.

A.2 Electrolysis Overview

¹⁶ For technologies whose typical hydrogen output pressure at gate is 1 MPa or lower, one can also report in addition to the 3 MPa, GHG emission at 1 MPa with the calculation result of GHG emission adjusted to 3 MPa which requires additional energy to increase the output pressure.



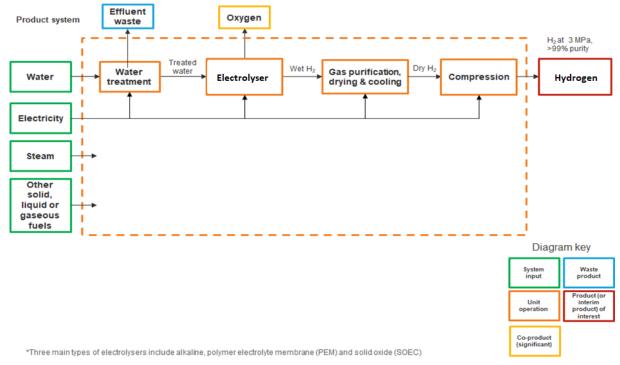


Figure 3: Process diagram for hydrogen produced from electrolysis

A.3 Emissions Sources in Electrolysis

GHG emissions associated with electrolysis are subject to the nature of electricity supply for electrolysis as electricity can be sourced from the grid (noting that this may be impacted by contracting of renewable electricity supply and associated instruments), generated on-site via the combustion of liquid, gaseous and/or solid fuels (in this case, this would be the key emissions source) or supplied from an off-grid on-site system.

Each process unit or stage in the electrolysis process contains emissions sources outlined in **Table 3**.

Table 3: GHG emissions summary for electrolysis

Process unit/stage	Key emissions sources	Other emissions sources	
Water supply and treatment	Electricity for purification		
	and filtration		
Hydrogen production	Electricity for electrolyser	Steam (where purchased) ¹⁷	
	units	Liquid, solid and/or gaseous	
		fuel combustion for steam	
		generation ¹⁸	
		Liquid, solid and/or gaseous	
		fuel combustion for	
		electricity generation ¹⁹	

¹⁷ Where high temperature SOEC are utilised



¹⁸ Where high temperature SOEC are utilised

¹⁹ Where on-site electricity generation is non-renewable

Hydrogen compression,	Electricity for relevant units	Steam (where purchased)	
purification, drying and		Solid, liquid and/or gaseous	
cooling		fuel combustion for relevant	
		units and/or steam	
		generation	

1 Allocation for the electrolysis pathway

Electrolysis system can be analysed as a single module (see **Figure 3**) with one co-product, oxygen that can be readily handled using prioritised coproduct management strategies (see Section 6.3.3.4). (i.e. system expansion). Energy allocation is not appropriate for this co-product, as oxygen does not have an energy content and zero emissions would be allocated to it using this method. Therefore, the use of system expansion is recommended for this co-product. Cryogenic distillation system is suggested as a substitute system for producing oxygen (the most common process for producing oxygen). This system separates air into oxygen, nitrogen and argon. Emissions associated with the oxygen product stream can be estimated referring to the air separation model established within the Ecoinvent life cycle database. These emissions may then be readily removed from the inventory if oxygen is sold to the market.

2 Information to be reported²⁰

Category	Matters to be identified	
Facility details	Facility identity	
	Facility location	
	Facility capacity	
	Commencement of facility operation	
Production	Production pathway	
Product specification	Hydrogen produced (kg)	
	Hydrogen pressure level at gate	
	Hydrogen purity level at gate	
	Specification of contaminants	
GHG emissions overview	Emissions intensity of hydrogen batch	
Batch details	Beginning and end of batch dates	
	Batch quantity	
Electricity	Location based emissions accounting:	
	Quantity of purchased grid electricity [kWh]	
	Location based emission factor used [kgCO₂e/kWh]	
	Market based emissions accounting	
	Quantity of purchased grid electricity [kWh]	
	Quantity of contracted renewable electricity [kWh]	
	and/or quantity of associated GOs or RECs	
	Type of GOs or RECs	
	Residual electricity	
	Residual mix emission factor [kgCO ₂ e/kWh]	

²⁰ In a country where GO system and residual mix system are not used for electricity emission counting, reporting of GO and residual mix related matters cannot be necessary.



On-site electricity generation	
Quantity of on-site generation [kWh]	
Emission factor for on-site generation (as applicable)	
[kgCO ₂ e/kWh]	
Source/s of water	
Source/s of steam	
Quantity of purchased water [kg]	
Quantity of purchased steam [kg]	
Quantity of steam exported [kg]	
Types of fuels combusted	
Quantities of fuel combusted [L, kg]	
Relevant emissions calculations and factors used	
Water treatment technology	
Electrolyser technology	
Hydrogen purification technology	
Water source/s	
Quantity of water used [kg]	
Quantity of oxygen produced [kg]	
Quantity of oxygen sold [kg]	
Emissions allocated to oxygen	

Appendix B Hydrogen Production Pathway – Steam Methane Reforming (With Carbon Capture and Sequestration)

B.1 SMR/CCS Process Description

Currently, the steam methane reformer (SMR) is the leading technology for H_2 production from natural gas or light hydrocarbons. In an SMR facility, GHG emissions are produced via combustion of fossil fuels for heat and steam, and via the reforming reaction. Modern SMR based hydrogen production facilities have achieved efficiencies that could reduce CO2 emissions down to nearly 10% above its theoretical minimum. Further reduction of CO2 emissions from hydrogen production would only be possible by the integration of CCS.

The base case consists of: (a.) feedstock pre-treatment, (b.) pre-reformer, (c.) primary reformer, (d.) high temperature shift reactor and (e.) pressure swing absorption or PSA.

The current industry standard for capturing CO2 from an SMR based H2 plant is the capture of CO2 from the shifted syngas using MDEA solvent. Four other CO2 capture options are considered as the use of H2 rich burner in conjunction with capture of CO2 from shifted syngas using MDEA; the capture of CO2 from PSA's tail gas using MDEA, or the use of Cryogenic and Membrane Separation; and the capture of CO2 from flue gas using MEA. These options involve the CO2 capture rate in the range of 56% to 90%.

The main simplified block flow diagram for a SME plant without CCS is described in Figure 4.

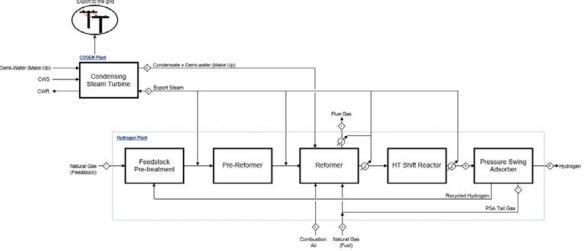
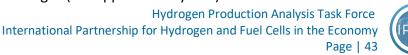


Figure 4: SMR plant without CO₂ capture.

Different technology options are available in the market to capture CO_2 from the different gas streams of the H_2 plant.ⁱⁱ

In this type of SMR plants, all of the CO_2 is emitted from the flue gas of the steam reformer. However, it should be noted that the CO_2 is produced from the following processes:

- CO₂ produced during the reforming and water-gas shift reaction;
- CO₂ produced during the combustion of the residual CO in the PSA tail gas and the natural gas (as supplementary fuel) in the SMR furnace.



B.2 SMR/CCS Overview

Depending on the available data, analysis can be performed across two different approaches to consider the delivery of the gas for steam methane reforming: (i) by using a well-documented emission factor of the gas purchased, (ii) by developing the upstream part (module 1) as follows.

Module 1 (upstream system) covers upstream activities associated with the extraction, processing and delivery of the natural gas feedstock. Potential co-products from the gas extraction and processing steps include natural gas liquids such as ethane, propane, butane and pentane, as well as oil and condensates. These products often co-exist with the gas extracted from the reservoir and are typically separated out from the gas stream as they attract a higher value when sold as separate products.

System expansion is not feasible for this application as an appropriate alternative method for producing these products does not exist. Therefore, allocation will be performed for these co-products based on the proportion of energy content (LHV) of the individual products.

The net remaining emissions are carried with the gas product stream (as embodied emissions) into the steam methane reforming system (module 2).

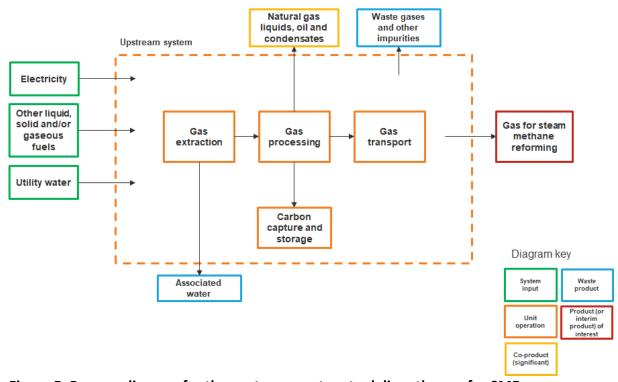


Figure 5: Process diagram for the upstream system to deliver the gas for SMR

Module 2 (steam methane reforming system)

The base case consists of: (a) feedstock pre-treatment (heating and pressurization), (b) pre-reformer (desulphurization), (c) primary reformer (SMR), (d) high temperature shift reactor and (e) pressure swing absorption (PSA).



For the SMR system (module 2), the only co-products are electricity, steam and/or carbon monoxide (pending the nature of the individual production facility).

Module 2: Steam methane reforming system

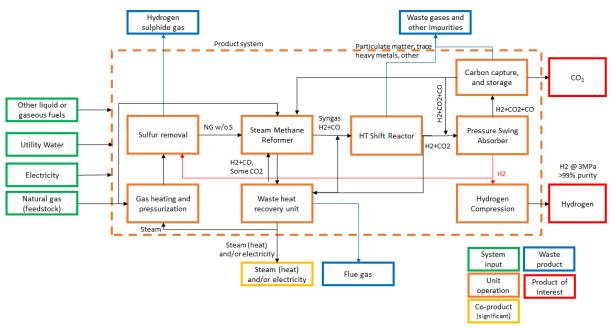


Figure 6: Process diagram for hydrogen produced from SMR/CCS

B.3 Emissions Sources In SMR/CCS

For steam methane reforming with CCS, the main source of GHG emissions is the conversion of natural gas (NG) to CO₂. Other significant emissions sources include the scope 2 emissions of grid electricity, CO₂ removal, CO₂ compression for CCS.

Each process unit or stage in the SMR process contains unique emissions sources as outlined in **Table 4**.

Table 4: GHG emissions summary for SMR /CCS

Process unit/stage	Key emissions sources	Other emissions sources
Natural gas processing	 Electricity and/or liquid fuel combustion for NG extraction and movement Fugitive methane and/or carbon dioxide from NG extraction 	
NG transport	 Electricity and/or liquid fuel combustion for materials movement 	



	Methane leakage	
Heat recovery and electricity generation	 No significant emissions other than those covered under common emissions sources 	
Hydrogen enrichment	 Water gas shift reactions occurring as part of hydrogen enrichment 	
Syngas purification	 Electricity and/or heat for operation of the relevant purification units 	 Exhaust CO₂ due to sulphur removal of exhaust gases (where applicable)
CO ₂ capture and separation	 Electricity and/or heat for relevant separation units Capture rate 	
Compression and transportation of CO ₂	 Electricity for compression of CO₂ Electricity and/or gaseous fuel combustion for pipeline transport Liquid and/or gaseous fuel combustion for motive transport Fugitive carbon dioxide from CO2 compression and transportation 	
Storage of CO ₂	Electricity for injection or transformation	 Fugitive CO₂ from permanent storage location
Hydrogen compression and storage	 Electricity for compression and storage maintenance 	 Fugitive hydrogen emissions²¹

B.4 Allocation for the SMR/CCS Pathway

Several co-products may exist for a SMR/CCS system. Steam, electricity, and a captured CO₂ stream are introduced as examples, but exact coproducts are representative of specific designs. If steam is exported from the system, the appropriate comparison system should

²¹ The impacts of hydrogen as an indirect GHG have not been considered as part of this work given current focus on (direct) GHG emissions accounting.



be based on the representative steam production process within the geographical region of interest. For a system expansion approach to allocation, steam, combustion of natural gas within a boiler has been identified as the dominant technology (currently) for generation of high-grade steam (heat).

Using steam production form a natural gas boiler, the GHG emissions assigned to steam is calculated considering:

- the quantity of NG needed to produce the quantity of steam (efficiency of the corresponding NG fired boiler that would produce the same quantity of steam)
- the residual (after CO₂ capture) GHG footprint (direct + indirect) of the above quantity of NG.

As such, if steam is exported from the system, allocation by energy is applied to calculate the associated CO_2e emissions.

If electricity is exported from the system, allocation by energy is applied to calculate the associated CO_2e emissions.

Allocation by energy is applied to calculate the energy use and CO₂e emissions of the supply of by-product H₂ from a CO plant.

CO₂ capture and underground storage is considered as a CO₂ removal.

B.5 Information to Be Reported²²

Category	Matters to be identified		
Facility details	Facility identity		
	Facility location		
	 Facility capacity (Nm³/h, t/h) 		
	Capacity Factor		
	Commencement of facility operation		
	 Main climatic and meteorological data 		
	(Atmospheric pressure, average ambient		
	temperature, average relative humidity)		
Production	Production pathway		
	 Product Specifications (H2 pressure, purity, 		
	contaminants)		
	 Quantity of hydrogen (kg) 		
GHG emissions overview	 Emissions intensity of hydrogen batch 		
	[kgCO ₂ e/kgH ₂]		
	 Type of offsets used (if applicable, noting that 		
	at this stage permitting the use of offsets is		
	contentious and not recommended)		

²² In a country where GO system and residual mix system are not used for electricity emission counting, reporting of GO and residual mix related matters cannot be necessary.



	 Quantity of offsets used (if applicable, noting that at this stage permitting the use of offsets is contentious and not recommended) 		
Batch details	Beginning and end of batch datesBatch quantity		
Electricity	 Location based emissions accounting Quantity of purchased grid electricity [kWh] Location based emission factor used [kgCO₂e/kWh] Quantity of sold electricity [kWh] 		
	 Market based emissions accounting Quantity of purchased grid electricity [kWh] Quantity of contracted renewable electricity [kWh] and/or quantity of associated GOs or RECs Residual electricity [kWh] Residual mix emission factor [kgCO₂e/kWh] Type of GOs or RECs 		
	On-site electricity generation • Quantity of on-site generation [kWh] • Emission factor for on-site generation (as applicable) [kgCO₂e/kWh]		
Other utilities	 Source/s of water Source/s of steam Quantity of purchased water [kg] Quantity of purchased steam [kg] Quantity of steam exported [kg] 		
Fuel feedstock	 Types of fuels combusted Quantities of fuel combusted [L, kg] Relevant emissions calculation or factors used [kgCO₂e/relevant unit of fuel] 		
Process	 SMR reactor type Syngas purification technology Sulphur waste gas processing technology (if applicable) Quantity and type of vented GHG gases [kg] Quantity and type of flared GHG gases [kg] Technology for monitoring fugitives from CO₂ storage CO₂ capture rate of the unit 		
Natural gas feedstock	 Type of NG NG composition 		



	 Quantity of NG used for SMR reactions [kg] Quantity of NG used for heating [kg] Quantity of NG used for producing steam [kg] Embodied emission factor for NG [CO₂e/kg] (derived from primary and secondary data, provided by supplier or sourced from relevant source i.e. NGA Factors)²³
Carbon dioxide treatment	 Type of CO₂ storage Location of CO₂ storage Transport type of CO₂ to storage location (if applicable) Quantity of CO₂ captured [kg] Quantity of CO₂ stored [kg] Quantity of fugitive emissions created during injection of CO₂ into the storage location [kg] Quantity of fugitive CO₂ emissions from storage [kg] (in line with period covered by the reporting)

²³ Note that where upstream emissions are derived using upstream data, there may be a requirement for additional information. This could include items such as coal source.

Appendix C Hydrogen Production Pathway – Industrial By-Product

C.1 By-Product Process Description

Chloralkali industry

There are 3 main processes: mercury cell, diaphragm cell and membrane cell. Membrane cell process is the most recently developed process (1970s) and is the most economic and environmentally-friendly process [Hung, et al., 2017]. The membrane process is used in 83.3% of chlor-alkali plants in the EU [Eurochlor, 2020] and is the only process still operational in the Netherlands [Scherpbier and Eerens, 2020]. As of 2019 there are no mercury plants operational anymore in the EU [Eurochlor, 2020]. The remaining plants are diaphragm (11.6%) and others (5.1%) (including chlorine and caustic soda production without hydrogen as a by-product) [Eurochlor, 2020]

In the EU, 9.4 Mton chlorine was produced in 2019 [Eurochlor, 2020]. With 28.4 kton H_2 produced per Mton chlorine with the membrane process [Scherpbier and Eerens, 2020] this corresponds to around 250 kton H_2 produced as a by-product in 2019 from membrane and diaphragm plants.

Worldwide there are at least 400 chloralkali plants, with a production capacity of 75 Mton chlorine per year [World Chlorine Council, 2017]. This corresponds to up to 2.1 Mton H_2 production per year (assuming all plants use membrane technology) Hydrogen can either be sold (merchant hydrogen) for industrial non-energy applications or used as fuel [Hung, et al., 2017]. Since 2002, 85-90% of the produced hydrogen in the EU is used [Eurochlor, 2020].

Process description by-product hydrogen production from the Chloralkali process

- The chloralkali process is an industrial process for the electrolysis of sodium chloride (NaCl) solutions. It is the technology used to produce chlorine (Cl₂) and sodium hydroxide (NaOH, caustic soda) which are commodity chemicals required by industry. Next to these main products for every mole of chlorine produced, one mole of by-product hydrogen is produced. Currently, much of this hydrogen is used to produce hydrochloric acid, ammonia, hydrogen peroxide, or is burned for power and/or steam production.
- Saturated (NaCl solution) brine enters the electrolysis cell at the anode side where the chloride ions are oxidized at the anode, losing electrons to become chlorine gas:

$$2Cl^- \rightarrow Cl_2 + 2e^-$$

 At the cathode, positive hydrogen ions pulled from water molecules are reduced by the electrons provided by the electrolytic current, to hydrogen gas, releasing hydroxide ions into the solution:

$$2H_2O + 2e^- \rightarrow H_2 + 2OH^-$$

• The ion-permeable membrane/diaphragm at the center of the electrolysis cell allows the sodium ions (Na+) to pass to the cathode side where they react with the hydroxide ions to produce caustic soda (NaOH). The overall reaction is:



$$2NaCl + 2H2O \rightarrow Cl2 + H2 + 2NaOH$$

Technology improvements can have an impact on the amount of hydrogen produced and the energy required for electrolysis, thereby having an impact on the emission factor for hydrogen

Zero-gap membranes decrease the distance between the anode and the cathode, reducing electrical resistance and heat production. Energy savings using zero-gap technology are ~10% [Scherpbier and Eerens, 2020]. This technology has become widespread since 2010, but due to high investment costs not all plants have converted yet.

Instead of producing hydrogen at the cathode, an oxygen depleted cathode ($ODC^{24,25,26,27}$) can be used – replacing the production of hydrogen by the use of oxygen. ODC reduces the required electricity for electrolysis by 30-40%, but the savings do not weigh up to the reduced income from hydrogen sales [Scherpbier and Eerens, 2020].

2 NaCl +H₂O + 0.5 O₂
$$\rightarrow$$
 2 NaOH + Cl₂ In formula form:

Steam cracking

Naphtha is the dominant feedstock for steam crackers, although steam cracking of ethane has become more attractive due to developments in shale gas extraction [Amghizar, et al., 2017].

With ethane as feedstock, hydrogen share in products is higher: 4% by mass [Lee and Elgowainy, 2018].

Annual production of ethylene is roughly 150 Mton (80 Mton propylene), naphta steam cracking representing roughly 10% of this [Amghizar, et al., 2017]

Which roughly translates to 350-450 kton hydrogen production from naphta steam cracking

In the US total potential hydrogen production from steam cracking is estimated to be 3.5 Mton hydrogen per year – 55% from existing plants and 45% from planned plants [Lee and Elgowainy, 2018]

Hydrogen produced in steam crackers is typically used as combustion fuel for the cracker, mixed with methane that is also produced as by-product or is imported from the grid [Lee and Elgowainy, 2018]

Process description by-product hydrogen production from (naphtha) Steam Cracking:

Moussallem, I., Jorissen, J., Kunz, U., Pinnow, S., Turek, T. (2008); Chlor-alkali electrolysis with oxygen depolarized cathodes: history, present status and future prospects, J Appl Electrochem (2008) 38: 1177-1194
 S. Bechtela, T. Vidakovic-Kocha, K. Sundmachera, Novel process for the exergetically efficient recycling of chlorine by gas phase electrolysis of hydrogen chloride, Chemical Engineering Journal 346 (2018) 535–548
 J. Jung, S. Postels, A. Bardow, Cleaner chlorine production using oxygen depolarized cathodes? A life cycle assessment, Journal of Cleaner Production 80 (2014) 46-56



²⁴ Chavan & Turek (2015); Chavan, N., Turek, T., Non-isothermal model for an industrial chlor-alkali oxygen depolarized cathode, Journal of Applied Electrochemistry (2015)

- Steam cracking of naphtha is used to generate olefins, e.g. for the production of
 plastics. First, naphtha is pre-heated to a temperature of 550-600°C while steam at a
 temperature of 180-200°C is added. Then, the naphtha is heated up to a
 temperature of 800-850°C where the hydrocarbon chains are cracked into ethylene
 and propylene as main products as well as various other compounds as by-products,
 thereof about 1% hydrogen by mass, or 2.63% by energy.
- The following table shows the yield of products and its composition for a typical steam cracking plant [CertifHy 2015].

Product	Share (%-energy)	Energy stream (TJ/yr)	
H ₂	2.63%	358	
СО	0.01%	1	
CH ₄	16.34%	2,226	
C ₂ H ₂	0.70%	96	
C ₂ H ₄	31.14%	4,242	
C ₂ H ₆	3.46%	471	
C ₃ H ₆	15.80%	2,152	
C ₃ H ₈	0.37%	51	
C ₄ H ₈	9.15%	1,246	
Pyrolysis gasoline	17.69%	2,410	
Pyrolysis fuel oil	2.69%	367	
Total	100.00%	13,622	

Figure 7. Yield and Product Composition of a Typical Steam Cracking Plant

C.2 By-Product Overview

The flow diagram of the chloralkali process is presented in Figure 8.

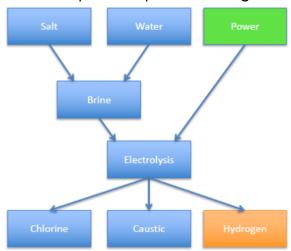


Figure 8: Process diagram for hydrogen produced from chloralkali process

The flow diagram of steam cracking is presented in Figure 9.

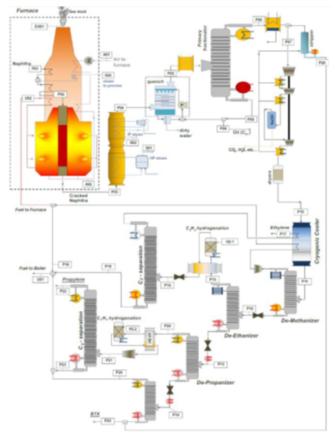


Figure 9: Process diagram for hydrogen produced from steam cracking

of importance is how the hydrogen is used. In this example $^{\sim}2/3$ of hydrogen is used as part of the fuel gas for the furnace (U02) and 1/3 is part of fuel gas used to fire a boiler (U01). [Spallina, et al., 2017].

C.3 Emissions Sources in By-Product

Chloralkali industry

The main emissions from the chloralkali production process are energy-related emissions. To produce a million tonnes of chlorine approximately 10 PJ of energy input is required, 1.9 PJ heat and 8.2 PJ electricity (see **Figure 10**).

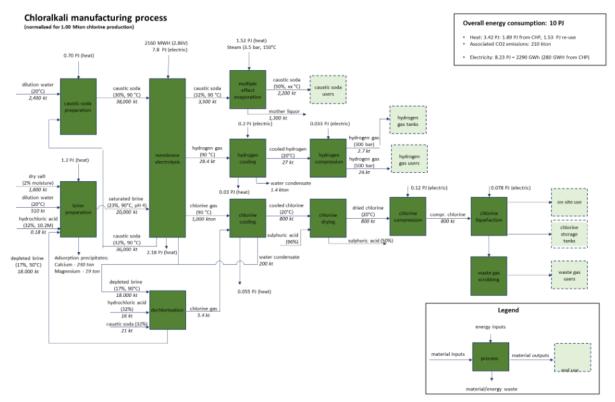


Figure 10: Energy diagram for the chloralkali process [Scherpbier and Eerens, 2020]

Other indirect emissions from the chloralkali process include emissions from salt (NaCl) mining and purification. 175 kg of NaCl is required as input per gigajoule hydrogen produced [CertifHy 2015].

Steam cracking

Emissions from steam cracking are related to the combustion of fuel gas used to provide the required heat to the process. Combustion occurs at the furnace and boilers (see for example **Figure 9**). The emissions depend on the feedstock used in the steam cracking process (naptha, ethane, propane, butane, or gasoil).

C.4 Allocation for The By-Product Pathway

Chloralkali industry

Six allocation methods were explored for hydrogen production as a by-product in the chloralkali sector. The results are presented in **Table 6**.

Enthalpy-based allocation was explored by the CertifHy project, resulting in an allocation factor for hydrogen of 52.9% [CertifHy, 2015].

Table 5: Electricity consumption for the production of hydrogen from chloralkali electrolysis.

	Unit	Allocation by energy	
Before allocation	kWh/kg _{H2}	80.75	
	kWh/kWh _{H2} , LHV	2.4233	
Allocation factor		52.9%	
After allocation	kWh _e /kWh _{H2, LHV}	1.2822	

Mass-based allocation is based on mass balances from Scherpbier and Eerens (2020). For every Mton chlorine, 1.1 Mton caustic soda and 28.4 kton hydrogen are produced (see **Figure 10**, where caustic soda is 50% diluted). Leading to a hydrogen share in the mass balance of \sim 1%.

Market value-based allocation was also explored by the CertifHy project, where an allocation factor of 11% was found [CertifHy, 2015]. Scherpbier and Eerens (2020) find a lower factor of 9% for the Netherlands. In Japan the market-value based allocation method leads to an allocation factor of 13%.

The CertifHy project also explored an allocation method based on the energy savings provided by the ODC process, where hydrogen is not produced as a co-product. The emissions of the co-produced hydrogen are the indirect emissions of the electricity that would be saved if the ODC process was implemented. It was assumed that energy savings amount to 25%, based on supplier information. This is corrected for the electricity required to produce oxygen (4.1%), resulting in an allocation factor of 20.9%.

For the substitution method It is assumed that every MJ hydrogen used for heat in the chloralkali process is replaced by 1 MJ natural gas. The Dutch natural gas emissions intensity of $56.8 \text{ g CO}_2/\text{MJ}$ is used.

Molar-based allocation is based on the molar fraction of hydrogen produced in the process (25%, with another 25% for chlorine and 50% for NaOH).

The hydrogen emissions intensity in **Table 6** are largely based on CertifHy (2015), where the intensity was determined based on the CO_2 intensity of the Dutch residual electricity mix and electricity from natural gas. Here we only use the CO_2 intensity of the residual mix in 2017 (642 gCO2e/kWh). With approximately 100 kWh required for 1 kg hydrogen. Scherpbier and Eerens (2020) base the emissions intensity on the total emissions from the chloralkali sector in the Netherlands. For the substitution method the natural gas emissions intensity in the Netherlands is used.

Table 6: Results of various emission allocation methods for hydrogen as by-product from the chloralkali industry.

Allocation Method	Share of emissions to be allocated to hydrogen	Hydrogen emissions intensity (g CO2e/MJ LHV H ₂)	Sources
Enthalpy-Based	53%	282	CertifHy (2015)
Mass-Based	1%	7	Own calculation



Market Value-Based	9-11%	34-59	Scherpbier and Eerens (2020) and CertifHy (2015)
Based on the energy			CertifHy (2015)
savings provided by	21%	134	Jung.(2014) and
the ODC process			Bechtel (2018)
Substitution	-	57	Own calculation
Molar-Based	25%	134	Own calculation

As energy-based allocation used in the other investigated pathways is not feasible, it is recommended for this first version to use the system expansion allocation based on the ODC process.

Steam cracking

Three allocation methods were explored for steam cracking. The findings are summarised in **Table 9**.

Energy-based allocation is based on findings from CertifHy (2015), with a hydrogen energy-share of 2.63%.

Lee and Elgowainy (2018) explored a substitution method, a mass-based allocation method and a market value-based allocation method. For the substitution method the share of hydrogen in the fuel gas depends on the feedstock used. Also dependent on the feedstock, natural gas to substitute hydrogen in fuel gas is either obtained from external sources or from the excesses in the tail gas. In the latter case, the amount of methane exported decreases. In all substitution cases, replacing hydrogen in fuel gas with methane increases the plant emissions. The authors estimate a WTG emission factor of $8.5-10 \text{ kg CO}_2/\text{kg}$ hydrogen, equivalent to $78-83 \text{ g CO}_2/\text{MJ}$ hydrogen.

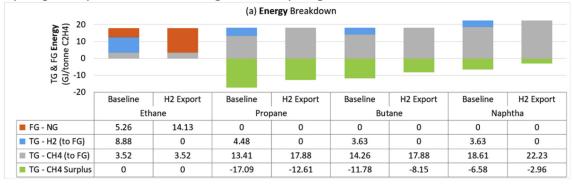


Fig. 3 – Breakdown of fuel gas (FG), a mixture of tail gas (TG, from steam crackers) and natural gas (NG, from the grid), flowing into a furnace as well as surplus methane (CH_4) in TG for two scenarios: baseline (hydrogen in TG is combusted in furnace) vs. H_2 export (hydrogen is exported to external market). Per 1 tonne of ethylene (C_2H_4) produced, energy intensity is the lowest (17.6 GJ/tonne C_2H_4) for ethane feedstock and highest (22.2 GJ/tonne C_2H_4) for naphtha. All in lower heating value (LHV).

Figure 11: Breakdown of fuel gas (FG)

Using mass or market value allocation methods also depend on feedstock used, as this determines the share of co-products from the steam cracker. The figure below shows the estimated emission factors are lowest for naphta steam crackers (just over 1 kg CO₂/kg H₂ or



8 g CO_2/MJ $H_2)$ and highest for ethane steam crackers (2-3 kg CO_2/kg $H_2)$.

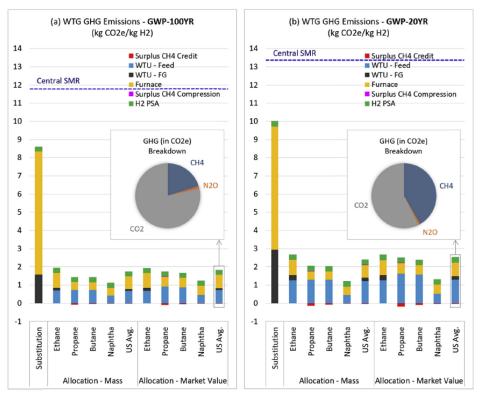


Fig. 5 – Life-cycle (well-to-gate) greenhouse gas emissions (in kg $CO_2e/kg\,H_2$) of by-product hydrogen production from steam crackers for substitution and allocation scenarios, by feedstock type (ethane, propane, butane, and naphtha), and U.S. average based on the weighting of production capacity (or feed slate). GHG emissions from the central SMR pathway, shown by dashed lines, are 12 kg CO_2e/kg hydrogen for GWP-100YR (left) and 13.4 for GWP-20YR (right).

Figure 12: Life-cycle (well-to-gate) greenhouse gas emissions

Wong and van Dril (2020) also assimilated data on the mass balance from steam cracking, based on the feedstock used. The hydrogen mass fraction is 0.5-2%, which is of a similar order of magnitude as the findings from Lee and Elgowainy (2018).

Table 7: Typical yield of co-products from feedstock's for steam cracking process (acc, 2004).

Product		Feedstock	
(kt)	Propane (LPG)	Naphtha	Gasoil
Ethylene	453.6	453.6	453.6
Propylene	166 - 296.5	199 - 222	183 - 196
Butadiene	18 - 32	56 - 77	76 - 82
Butenes/Butanes	13 - 22	60 - 128	78 - 88.5
Pyrolysis gasoline	47 - 71	183 - 494	294 - 342.5
Benzene	17 - 26.5	51 - 84	96 - 109
Toluene	5 - 5.5	19.5 - 71.5	51 - 54.4
C ₈ aromatics	0	26.5 - 43	20 - 43
Other	25 - 39	86 - 295	127 - 136
Fuel oil	4.5 - 10	29.5 - 51	289 - 376.5
Methane-rich gas	263 - 296.5	199 - 222	183 - 196
Hydrogen-rich gas	17 - 21	11 - 14	12 - 26.5
Total	982 - 1,200	1,173 - 1,670	1,614 - 1,822
Ethylene yield (%)	38 - 46	27 - 39	25 - 28

A market value-based allocation factor was also calculated based on the co-product mass balance from Wong and van Dril (2020) and European prices as given in Boulamanti and Moya (2017). Market values can differ significantly over time and across the world and the share allocation can be influenced by this.

Table 8: Market value-based allocation for hydrogen co-product from steam cracking based on Wong and van Dril (2020) and European co-product from Boulamanti and Moya (2017).

Product	Value (€/ton)	Propane (M€)	Naphta (M€)	Gasoil (M€)
Ethylene	748	339	339	339
Propylene	1008	117-299	201-224	184-197
Butadiene	885	16-28	50-68	67-73
Butenes/butanes	639	8-14	38-82	50-57
Pyrolysis gasoline	789	74-112	289-779	464-540
Fuel oil	468	2-5	14-24	135-176
Methane-rich gas	526	138-156	105-117	69-103
Hydrogen-rich gas	1344	23-28	15-19	16-36
Total	-	718-981	1050-1651	1352-1521
Hydogen share	-	3%	1%	1-2%

Table 9: Results of various emission allocation methods for by-product hydrogen from steam cracking.

			•
Allocation method	Share of	Hydrogen	Sources
	emissions to	emissions	
	be allocated	intensity (g CO ₂	
	to hydrogen	eq/MJ LHV H ₂)	



Energy-based	2.6%	21.8	CertifHy (2015)
Substitution	-	71-83	Lee and Elgowainy (2018)
Mass-based	0.5-4%	8-25	Wong and van Dril (2020),
			Lee and Elgowainy (2018)
Market value-based	1-3%	8-25	Wong and van Dril (2020),
			Boulamanti and Moya
			(2017), Lee and Elgowainy
			(2018)

As energy-based allocation is recommended for by-product hydrogen from steam cracking.

Appendix D Hydrogen Production Pathway – Coal Gasification (With Carbon Capture and Sequestration)

D.1 Coal Gasification/CCS Process Description

Coal is removed from coal seams using either open-pit or underground mining depending upon the depth of the coal seam. These operations consume electricity for conveying to and from storage areas and through the crushing and washing facilities.

The coal is transported to a processing facility via ships, trucks and trains. Loading and unloading steps typically employ electricity driven stackers/reclaimers and associated conveyors. Transport vessels use diesel, fuel oil or electricity for motive power.

To produce hydrogen gas, coal is mixed with oxygen and steam in a reactor (a gasifier). The basic gasification reaction is:

C (carbon, in coal) + H_2O (steam) + heat $\rightarrow CO$ (carbon monoxide) + H_2 (hydrogen)

The reaction takes place at high temperatures and some of the coal is oxidised by the oxygen to produce the energy needed to drive the reaction:

$$C+O_2$$
 (oxygen) $\rightarrow CO_2$ (carbon dioxide) + heat

The oxygen used in the gasifier is generated in an air separation unit. Oxygen is used in preference to air, to prevent nitrogen diluting and contaminating the hydrogen. Air separation technologies include cryogenic distillation, pressure-swing adsorption, and membrane separation. All consume large quantities of electricity. In addition to liquid oxygen and liquid nitrogen, crude liquid argon may also be produced in smaller quantities (argon constitutes about 0.93% of air) (Althaus, 2007). Pending the scale and valorisation of these outputs, they may be considered as co-products and allocated emissions.

A gasifier is a high temperature reactor where coal undergoes partial oxidation and reaction with steam. There are three main types of gasifiers that can be used to create syngas, each varying in the method it uses to generate heat, to contact the reactants and the physical state of the residue it produces. These are fixed bed (e.g. Sasol-Lurgi gasifiers), fluidised bed (e.g. Winkler gasifiers) and entrained flow (e.g. Koppers-Totzek gasifiers) (Kopp, 2000) (Higman, 2008). These different gasifiers have their advantages and disadvantages but at a macro level perform the same function. They have common inputs (coal, oxygen and water) but can produce syngas with varied properties, also subject to the properties of the coal, which will impact the configuration of downstream processing activities.

This unit also produces ash and/or slag as waste products.

Waste heat recovery units are typical for coal gasification processes, reflecting the high temperature operation of coal gasification processes and the requirement for cooling of syngas products for subsequent processing. Regulation of the gasifier temperature is



managed through a heat exchanger which can be used to raise steam and generate electricity. Steam may be supplied elsewhere in the plant (i.e. steam use in regeneration of acid gas removal (AGR) absorption systems) or exported out of the product system boundary. Electricity may be generated from this steam and used elsewhere in the plant such as to drive the air separation process, or exported beyond the product system boundary.

Any exported steam and/or electricity is considered a co-product and should be allocated a share of emissions.

Syngas conditioning

The output of the gasifier is a stream of raw syngas, which may contain a number of contaminants, including particulate matter and heavy metals. In addition, this stream contains significant CO gas. To maximise the quantity of hydrogen produced, syngas from the gasifier is sent through to another reactor where the carbon monoxide is reacted with water to yield additional hydrogen. This is known as the water-gas shift (WGS) reaction, as follows: $CO+H_2O \rightarrow CO_2+H_2+heat$. This is a reversible reaction, with an equilibrium established between CO and CO₂, subject to the reaction conditions. Low temperatures favour the formation of CO2. As the conversion of CO to CO₂ generates heat, there are often several water gas shift reactors in series with coolers between them (including high temperature and low temperature stages). Typically, iron-chromium and copper-zinc catalysts are used to facilitate the reaction at high and low temperatures, respectively (Pal, Chand, Upadhyay, & Mishra, 2018). High temperature WGS may include conversion of sulphur compounds to hydrogen sulphide (H2S), for removal in the acid gas removal (AGR) stage.

The syngas now includes large quantities of CO_2 in addition to other impurities including sulphur compounds (such as H_2S) and heavy metals (such as mercury). These components must be removed from the syngas. Particulate matter can be removed using a water scrubber. Mercury and other heavy metals can be removed by via adsorption, particularly using activated carbon beds. Drying (water removal) is also required (Higman, 2008). Sulphur compounds may be removed using lime. CO_2 and sulphur compounds can also be removed together. The capture of CO_2 and removal of these sulphur compounds simultaneously is discussed below.

Whilst configurations for syngas conditioning vary, the key inputs and outputs (electricity, heat) are largely common.

Carbon capture and storage (CCS)

Carbon capture, and storage (CCS) refers to the capture and storage of waste carbon dioxide in a geologic reservoir, for the purposes of reducing emissions of CO₂ to the atmosphere. The CCS stage consists of three main unit operations including separation and capture, compression and transport and storage or utilisation.

CO₂ capture and separation

Acid gas removal refers to the separation of H₂S and CO₂ (for carbon capture) via physical solvents (such as the SelexoITM system), chemical solvents (such as mono-ethanol amine



(MEA)), other means (such as pressure swing adsorption (PSA)) or some combination which reflects syngas properties and product output requirements. Removal of H₂S and CO₂ at a large scale is typically performed by passing the syngas through a counter-current absorption column with a regenerative solvent (physical or chemical). For pre-combustion carbon capture processes physical absorption is favoured given typically high CO₂ partial pressures (Vega, et al., 2018). To pump the solvent through the absorber and recover the solvent, heat exchangers, reboilers, coolers and pumps are required. Sulphur containing gas (particularly H₂S) from the regeneration unit is produced which may be processed into sulphur in a Claus plant (Chiche, Diverchy, Lucquin, Porcheron, & Defoort, 2013). This sulphur may be sold as a co-product. However, given the scale of this sulphur source and the requirement for additional processing, the H₂S stream is considered a waste stream. Although solvent absorption is the most common method of syngas purification, if the gas contains significant concentrations of other gases besides H₂ and CO₂, other methods may be preferred (Hofbauer, Rauch, & Ripfel-Nitsche, 2007). The two main alternative processes are pressure-swing adsorption (PSA) and cryogenic distillation. However, membrane separation has also gained a lot of attention in the last decade (Rezaee & Naeij, 2020), and several types of membranes are now available which can be used to produce hydrogen streams of very high purity (Scholes, Smith, Kentish, & Stevens, 2010). For the purpose of this work and at a macro level, the many capture processes and the corresponding complex unit operations can each be simply treated as units that separate hydrogen from carbon dioxide through the application of electricity and heat (typically low-grade).

CO₂ compression and transportation

Prior to transportation, the purified CO₂ gas must be pressurised. Selection and design of compressors should be reflective of both the condition and scale of the carbon capture and transport required (Martynov, Daud, Mahgerefteh, Brown, & Porter, 2016). Key inputs will be electricity to power compression, with petroleum oils and greases required for operation. This transport can occur in multiple ways including pipeline, road tankers, rail tankers and ships (National Research Council, 2007). For large volumes of CO₂, pipelines are generally the most economical form of transportation. Where pipelines are used, leakage rates must be considered across the length of the pipeline, subject to operating pressure.

Storage of CO₂

There are several ways the CO_2 can be stored permanently. In this case, the amount of CO_2 stored is considered as a removal (considering the associated emissions due to its separation, capture, compression, transport and storage).

There are currently two broad categories: the storage of gaseous CO_2 in geological formations and the reaction of CO2 to form stable minerals. There is also some interest in the use of biological matter (bacteria and algae) which degrade captured CO_2 over time. Geological storage typically involves the injection of supercritical CO_2 into deep underground geological formations such as oil and gas fields, unmineable coal seams and saline formations (Environmental and Energy Study Institute, 2020). CO_2 may also be dissolved in aquifer water, with saline aquifers of particular interest (given frequency and potential storage volume) (Environmental and Energy Study Institute, 2020). Mineral sequestration refers to the reaction of CO_2 to form stable minerals, particularly carbonates.



The Hydrogen Energy Supply Chain project in the Latrobe Valley is planning to establish a CCS network from the hydrogen production facility to offshore storage locations within the Gippsland Basin (HESC, 2020). There are a number of ancillary activities including modelling, drilling of monitoring wells, monitoring of the CO₂ plume throughout injection and long-term monitoring of sequestration sites for potential leakage (this may include subsurface monitoring, seismic monitoring, surface monitoring). Geological storage is of greater concern as mineral storage is not considered to have significant leakage risks.

Hydrogen compression and buffer storage

Common to hydrogen produced via coal gasification, electrolysis, and any other means is the requirement for compression of the dry, high purity hydrogen product. This is particularly important given the low density of hydrogen gas. Subject to the nature of downstream hydrogen storage, transport and use, there will be different requirements for hydrogen compression. Common to the coal gasification, electrolysis and steam methane reforming pathways, there are four main approaches to hydrogen storage: compressed gaseous hydrogen, liquid hydrogen and materials-based storage technologies (either physical or chemical).

With regards to hydrogen compression and storage, it is important to be clear about the boundary for certification. Where storage is required for the delivery of the functional unit (i.e. hydrogen under the specific boundary conditions) this must be included within the system boundary. However, where the hydrogen is processed (for storage or otherwise) in such a way as to provide additional functionality (e.g. the liquefaction of hydrogen for delivery to customer to meet their preferences) this should be treated using a module (or annex, yet to be developed) covering hydrogen energy carriers. Different forms of storage are briefly described below but their inclusion within the defined system boundary is subject to the considerations noted above.

Compression refers to the storage of hydrogen in its gaseous form at higher pressures. This includes pressurisation of hydrogen within steel cylinders but also includes large-scale and longer-term storage in locations such as salt caverns and depleted gas fields, and the storage of hydrogen in existing natural gas pipelines (line packing) (Makridis, 2016).

D.1 Coal Gasification /CCS Overview



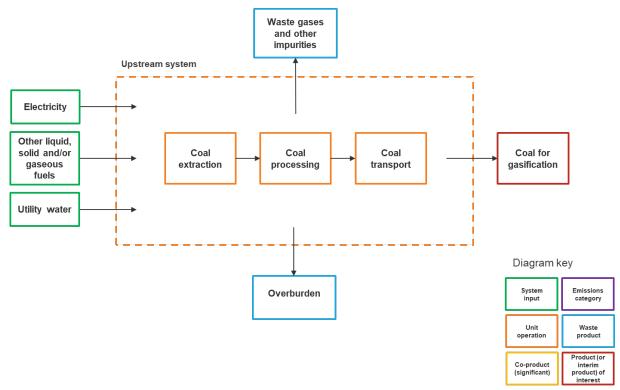


Figure 13: Coal gasification upstream system

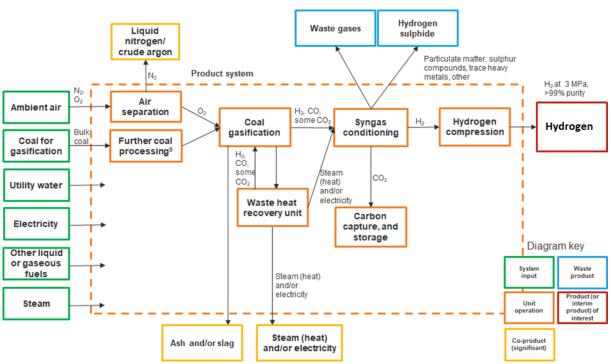


Figure 14: Coal Gasification system

D.3 Emissions Sources In Coal Gasification /CCS

For coal gasification with CCS, the main source of GHG emissions is the conversion of carbon in coal to CO₂. Other significant emissions sources include the scope 2 emissions of grid electricity used for air separation (including air compression and oxygen compression), CO₂

removal, CO₂ compression for CCS, coal processing (size reduction and cleaning) activities and fugitive methane emissions associated with coal mining.

Each process unit or stage in the coal gasification process contains unique emissions sources as outlined in

Table 10.

Table 10: GHG emissions summary for coal gasification /CCS

Process unit/stage	Key emissions sources	Other emissions sources
Coal mining and processing	Electricity and/or liquid fuel	Explosives for coal
	combustion for materials	extraction
	extraction and movement	
	Fugitive methane and/or	
	carbon dioxide from coal	
	extraction	
Primary coal processing	Electricity for loading and	Chemical usage for coal
	unloading of coal	processing
	Electricity for coal size	
	reduction, washing and	
	separation	
Coal transport	Electricity and/or liquid fuel	
	combustion for materials	
	movement	
Further coal processing	Electricity for additional size	Electricity and/or liquid fuel
	reduction	combustion for materials
		movement
Air separation	Electricity for air	
- 10	compression	
Gasification	Combustion of coal within	
	the gasifier	
	Gasification of coal within	
	the gasifier	
	Steam for gasification (if	
	purchased from third party	
Heat receivery and	rather than self-generated)	
Heat recovery and	No significant emissions other than those covered	
electricity generation	under common emissions	
Hydrogon oprichment	Sources Water gas shift reactions	
Hydrogen enrichment	Water gas shift reactions occurring as part of	
	hydrogen enrichment	
Syngas purification	Electricity and/or heat for	Exhaust carbon dioxide due
Syrigas purification	operation of the relevant	to sulphur removal of
	purification units	exhaust gases using lime
		(where applicable)
		(writere applicable)

CO2 capture and separation	Electricity and/or heat for	
	relevant separation units	
Compression and	Electricity for compression	
transportation of CO2	of CO2	
	Electricity and/or gaseous	
	fuel combustion for pipeline	
	transport	
	Liquid and/or gaseous fuel	
	combustion for motive	
	transport	
	Fugitive carbon dioxide	
	from CO2 transportation	
Storage of CO2	Electricity for injection or	Fugitive carbon dioxide
	transformation	from permanent storage
		location
Hydrogen compression and	Electricity for compression	Fugitive hydrogen
storage (if in the production	and storage maintenance	emissions ²⁸
boundary)		

D.4 Allocation for The Coal Gasification /CCS Pathway

The coal gasification production pathway has been divided into distinct modules to facilitate application of emissions accounting analysis through system expansion. For coal gasification, analysis is performed across three distinct modules, as follows:

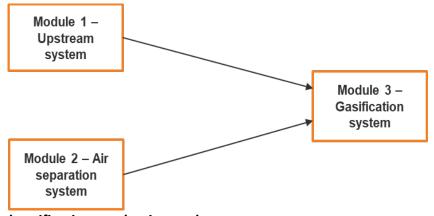


Figure 15: coal gasification production pathway

Module 1 (Upstream system) – covers upstream activities associated with the extraction, processing and delivery of the coal feedstock. This system is taken out of the process as a separate module to allow treatment of this system in different ways (i.e. collection of primary and secondary data²⁹ to derive a local or regional emission factor, or use of a scope

²⁸ The impacts of hydrogen as an indirect GHG have not been considered as part of this work given current focus on (direct) GHG emissions accounting.

²⁹ As per the GHG Protocol Standard "primary data are data collected from specific processes in the studied product's life cycle" and "secondary data are defined as data that are not from specific processes in the studied product's life cycle"

3 emission factor that should at a minimum be country specific³⁰). As this system has a single product, no emissions allocation approaches are required and all emissions are attributed to a single output, coal for gasification. That is, all emissions associated with this system are allocated to the intermediate product: coal. These emissions are carried with the coal (as embodied emissions) into the gasification system (module 3). Where applicable assessment of module 1 may be by-passed via use of an appropriate scope 3 emissions factor covering coal supply.

Module 1: Upstream System

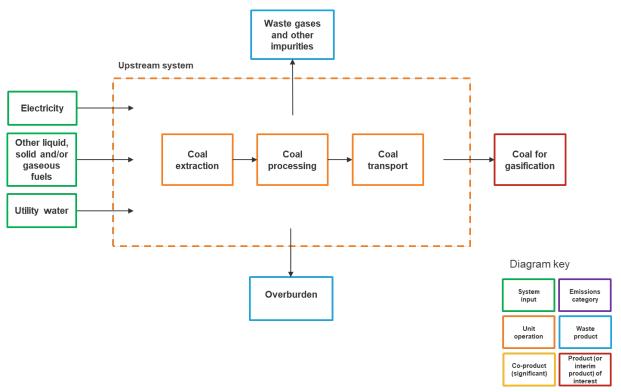


Figure 16: Coal gasification upstream system

Module 2 (Air separation system) – covers the supply of oxygen for the coal gasification process. For module 2, there are two potential co-products (liquid nitrogen and liquid crude argon) associated with the system in addition to the intermediate product: liquid oxygen³¹. This system has been scoped out for allocation as, unlike the remainder of the gasification system (module 3), it cannot be resolved using methods to avoid allocation³².

The liquid nitrogen stream will be significant given its abundance relative to oxygen in air and the oxygen demands of an industrial gasifier. The argon stream will be much smaller,

³⁰ Note this treatment is likely dependent on the availability of data. For an integrated system where the hydrogen producer extracts and processes coal, it is reasonable that they might wish to collect primary and secondary data to assess the upstream emissions and derive an embodied emission factor for their coal. However, if the coal is simply bought from a supplier this supplier may provide an embodied emission factor for this coal or in some cases a default embodied emission factor for coal may be identified in appropriate life cycle databases.

³¹ Some waste heat may also be produced as the electricity is consumed.

³² Process subdivision is not appropriate as the process unit cannot be broken down further. Functional unit expansion is not appropriate in the context of this work (as previously noted). System expansion is not appropriate as cryogenic air separation is a typical, system for largescale oxygen supply and a suitable alternative system is not available.

reflecting the low argon concentration in air (approximately 0.93%). One or more of these co-products may be captured and sold noting that they have a variety of common uses. Where these co-products are valorised they may be allocated some share of emissions. The priority approach is to allocate on the basis of physical relationships. The Ecoinvent database's *Life Cycle Inventories of Chemicals* outlines an approach for allocation of emissions across the three liquid products on the basis of the heat of vaporisation and heat capacity of the three liquid products assuming that the thermodynamic efficiency of the cooling and liquefaction process is the same for all three gases (Althaus, 2007). This results in an allocation factors of 22.2% for oxygen, 76.9% for nitrogen and 0.9% for crude argon.

Emissions associated with the intermediate oxygen product can be estimated as follows:

Eliquid oxygen=Eair separation-Eliquid nitrogen-Eliquid crude argon

Where $E_{liquid\ oxygen}$ is the emissions associated with liquid oxygen, E_{air} separation is the total emissions associated with the air separation module (as calculated in line with the guidance provided for module emissions inventories), and E_{liquid} nitrogen and $E_{liquid\ crude\ argon}$ are the emissions associated with the co-products as calculated using the allocation factors referred to above.

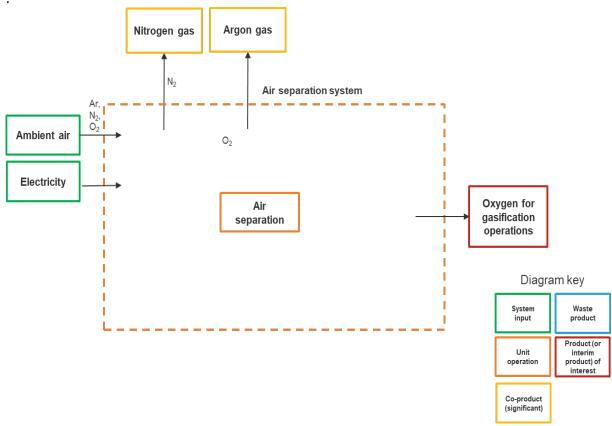


Figure 17: Air separation system

Module 3 (Gasification system) – covers all remaining processes including further coal processing, gasification, syngas conditioning and waste heat recovery.



For module 3, inputs include the intermediate products from modules 1 and 2, which carry an emission factor (reflecting embodied emissions).

The gasification system includes a range of potential co-products, including electricity and steam, generated via waste heat recovery, ash and/or slag recovered from the gasifier and sulphur recovered via syngas purification. The scale of production for these potential co-products remains uncertain and is likely subject to facility-specific commercial circumstances (i.e. energy costs, grid considerations, plant design and operation).

Where applicable, emissions may be scoped out for the co-products using system expansion. In order to do so, appropriate substitute systems must be identified and appropriate allocation factors established.

Electricity is likely to be an important co-product for the gasification system. Electricity exported from the system could substitute grid electricity (kWh for kWh), and emissions estimated in line with relevant grid emission factors (i.e. local, regional, national). This is a common approach in various carbon accounting schemes. Energy allocation could also be applied to this co-product.

Steam may also be an important co-product for the gasification system, but this is likely to be highly dependent on the availability of appropriate infrastructure and nearby consumers given the nature of steam supply. Currently the dominant technology for generation of highgrade steam (heat), is via combustion of natural gas within a boiler. As such, steam exported from the system could be estimated in line with the emissions associated with equivalent steam produced in a natural gas boiler of a pre-defined default efficiency (ARENA, 2016).

The ash and slag products are significantly less material. Default allocation factors should be defined here relating to appropriate substitute systems. For ash and slag, these co-products vary in uses from low-value applications such as replacing natural aggregates to high-value applications such as replacing clinker in cement production. A conservative emission factor should be established as the default, but it may be important to include measures which allow and incentivise users of the scheme to seek out higher quality data specific to their value chain.

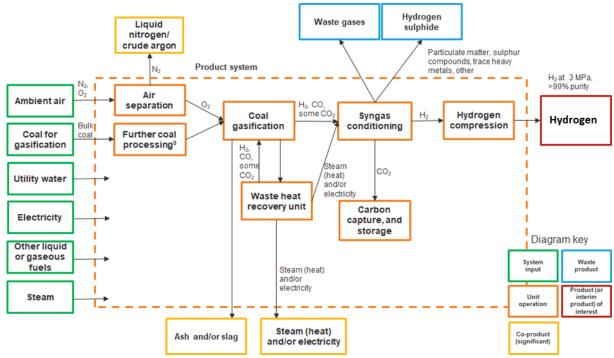


Figure 18: Coal Gasification system

D.5 Information To Be Reported³³

Category	Matters to be identified
Facility details	Facility identity
	Facility location
	Facility capacity
	Commencement of facility operation
Production	Production pathway
Product specification	Hydrogen output pressure
	Hydrogen purity
	Contaminants
	Hydrogen quantity (kg)
GHG emissions overview	Emissions intensity of hydrogen batch
	Type of offsets used (if applicable, noting that at this
	stage permitting the use of offsets is contentious and
	not recommended)
	Quantity of offsets used (if applicable, noting that at
	this stage permitting the use of offsets is contentious
	and not recommended)
Batch details	Beginning and end of batch dates
	Batch quantity
Electricity	Location based emissions accounting

³³ In a country where GO system and residual mix system are not used for electricity emission counting, reporting of GO and residual mix related matters cannot be necessary.



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	Quantity of purchased grid electricity [kWh]
	Location based emission factor used [kgCO ₂ e/kWh]
	Market based emissions accounting
	Quantity of purchased grid electricity [kWh]
	Quantity of contracted renewable electricity [kWh]
	and/or quantity of associated GOs or RECs
	Residual electricity [kWh]
	Residual mix emission factor [kgCO ₂ e/kWh]
	Type of GOs or RECs
	On-site electricity generation
	Quantity of on-site generation [kWh]
	Emission factor for on-site generation (as applicable)
	[kgCO ₂ e/kWh]
Other utilities	Source/s of water
	Source/s of steam
	Quantity of purchased water [kg]
	Quantity of purchased steam [kg]
	Quantity of steam exported [kg]
Fuel feedstock	Types of fuels combusted
	Quantities of fuel combusted [L, kg]
	Relevant emissions calculation or factors used
	[kgCO ₂ e/relevant unit of fuel]
Process	Coal gasification reactor type
	Syngas purification technology
	Air separation technology
	Sulphur waste gas processing technology (if
	applicable)
	Quantity and type of vented GHG gases [kg]
	Quantity and type of flared GHG gases [kg]
	Technology for monitoring fugitives from CO ₂ storage
	CO ₂ capture rate
Coal feedstock	Type of coal
	Coal composition
	Quantity of coal used for gasification reactions [kg]
	Quantity of coal used for heating [kg]
	Embodied emission factor for coal [kgCO ₂ e/kg]
	(derived from primary and secondary data, provided
	by supplier or sourced from relevant source i.e. NGA
	Factors) ³⁴
Carbon dioxide treatment	Type of CO ₂ storage
	Location of CO ₂ storage

³⁴ Note that where upstream emissions are derived using upstream data, there may be a requirement for additional information. This could include items such as coal source.



	Transport type of CO ₂ to storage location (if
	applicable)
	Quantity of CO ₂ captured [kg]
	Quantity of CO ₂ stored [kg]
	Quantity of fugitive emissions created during injection
	of CO₂ into the storage location [kg]
	Quantity of fugitive CO ₂ emissions from storage [kg]
	(in line with defined timeline)
Waste and/or co-products	Quantity of ash produced [kg]
	Quantity of slag produced [kg]
	Quantity of nitrogen produced [kg]
	Quantity of crude argon produced [kg]
	Quantity of ash sold [kg]
	Quantity of slag sold [kg]
	Quantity of nitrogen sold [kg]
	Quantity of crude argon sold [kg]
	Quantity of other products [kg]

Bibliography

ⁱ GHG protocol Scope 2 Guidance (2015)

https://ghgprotocol.org/sites/default/files/standards/Scope%202%20Guidance Final Sept26.pdf

ⁱⁱ IEAGHG, "Techno-Economic Evaluation of SMR Based Standalone (Merchant) Plant with CCS", 2017/02, February, 2017

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