

New technologies and strategies for fuel cells and Hydrogen Technologies in the phase of recycling and dismantling

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D4.2 LCA of materials represented in FCH technologies

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Executive Summary

The scope of this document is to assess materials used in considered technologies from environmental point of view by using the approach to Life Cycle Analysis (LCA) defined in deliverable D4.1 [1]. The critical materials in considered Fuel Cells and Hydrogen (FCH) technologies were revised in D2.1 [2] and the EoL processes in D2.2 [3], D3.1 [4], and D3.2 [5].

First, the materials are listed and identified according to considered FCH technology (PEMFCs, SOFCs, AWEs and PEMWEs). They are classified according to their criticality, their presence in life cycle assessment databases and general availability in those databases and at the end associated to the appropriate End of Life (EoL) processes.

For the LCA study Thinkstep Gabi software was used with Gabi professional database and Ecoinvent 3.3 database, [6], [7]. The methodology used for Life Cycle Impact Assessment (LCIA) was midpoint CML2001 methodology, [8], [9]. Materials in the production stage are evaluated per 1 gram of material as an input flow into manufacturing process of considered FCH technology. Result of each environmental impact indicator is normalized according to the material that exhibits the lowest value. This way all the materials are ranked proportionally to the least harmful material. To identify potentially most critical (environmentally harmful) materials, the results are also sorted according to each considered FCH technology with separated results for balance of plant (BoP) components.

In next steps the mass ratio of materials for each considered technology will have to be defined in order to get results of environmental impacts of each considered technology. With the available and future end of life recycling technologies environmental impacts of each considered technology will be additionally evaluated.



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Abbreviations

AWE	Alkaline Water Electrolyser
BoP	Balance of Plant
EL	Electrolyser
ELCD	European reference Life Cycle Database
EoL	End of Life
EoLA	End of Life Assessment (Analysis)
EPLCA	European Platform on Life Cycle Assessment
FC	Fuel Cell
FCH	Fuel Cell and Hydrogen
FCH-JU	Fuel Cell and Hydrogen Joint Undertaking
HDPE	High Density Polyethylene Granulate
ILCD	International Reference Life Cycle Data System
LCA	Life Cycle Analysis
LCC	Life Cycle Costs
LCDN	Life Cycle Data Network
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
MEA	Membrane Electrode Assembly
PEEK	Polyether ether ketone
PEM	Polymer Electrolyte Membrane
PEMEC	Polymer Electrolyte Membrane Electrolyser Cell
PEMFC	Polymer Electrolyte Membrane Fuel Cell
PEMWE	Polymer Electrolyte Membrane Water Electrolyser
PFSA	Perfluorosulphonic acid (Nafion)
PGM	Platinum group metal
PTFE	Polytetrafluoroethylene (Teflon)
SOFC	Solid Oxide Fuel Cell



1. Introduction

One of the near term possibilities to decarbonize energy and transport sectors in the EU is successful commercialization of fuel cells and hydrogen (FCH) technologies. The idea is to generate vast amounts of green hydrogen from the expected surplus of renewable energy sources (implemented policies are going towards 65% of electricity from renewable energy sources by 2050) to be used in transport, energy and industries. However, most widely used commercial FCH technologies, which are also taken into consideration in this project (PEM and alkaline electrolysers as well as PEM and solid oxide fuel cells) are not fully prepared for deployment yet due to insufficient infrastructure and certain societal barriers. Wide deployment of commercial FCH technologies is also conditioned by lack of well-defined end-of-life (EoL) strategies. Within this context, the HyTechCycling project aims to deliver reference documentation and studies on both conventional and novel EoL technologies and strategies applicable to FCH technologies, paving the way for future demonstration actions and advances in roadmaps and regulations.

As part of the project, a Life Cycle Assessment (LCA) study has to be carried out for all life cycle phases for the considered FCH technologies with particular emphasis on the EoL phase. The recycling and dismantling stage is of key importance for successful commercialization of FCH technologies. Up till now nearly all of LCA studies have disregarded the EoL stage of these products. To successfully carry out the LCA study a proper software environment, methodology, and relevant key components (materials) of the considered FCH technologies were defined in D2.1, [2]. Further, impact criteria, boundary conditions of the LCA study, functional unit and other relevant data required for the LCA study were defined in D4.1, [1]. The present report addresses the LCA analysis of most widely used materials in the considered FCH technologies.

The goal is to carry out the LCA and LCIA of all the materials in considered technologies. Since we are dealing with rather new materials, some of them are still not available in LCA databases. Within first part of the LCA study the materials in their production phase, from the mine to the beginning of the FCH technology manufacturing phase, were assessed. The results partly correspond to criticality assessment method presented in D2.1, [2], but they are much more detailed since different environmental criteria are assessed. In the next step materials are linked with dismantling and recycling processes that are already commercially/industrially available or are just small scale (laboratory) processes not yet established in the industry, [3]. To make LCA of these processes, they need to be in the LCA databases or will have to be defined with appropriate LCIA approach for further assessment.



2. Identification of critical materials

Within this task majority of work was done in D2.1 [10], where the most critical materials were identified using the procedure shown in Figure 1.



Figure 1: Procedure for identification of critical materials.

Four FCH technologies taken under consideration in the HyTechCycling project are alkaline water electrolyser (AWE), polymer electrolyte membrane water electrolyser (PEMWE), polymer electrolyte membrane fuel cell (PEMFC), and solid oxide fuel cell (SOFC). These technologies were broken down to main components that comprise them in order to identify most commonly used materials. Among these materials the critical materials were identified using the methodology explained below.

2.1 Methodology for criticality assessment of materials

Three main criteria were defined for classification of most commonly used materials in the FCH technologies. These criteria include hazardousness, scarcity or criticality, and price or value of the materials, [2].

2.1.1 Hazardous materials waste

In this project different references were used to determine material hazardousness of the most commonly used materials in FCH technologies: The Priority List of Hazardous Substances [11], [12], [13], and report from Robert A. Goyer and Thomas W. Clarkson about toxic effects of metals, [14].

2.1.2 Scarce or critical materials in the supply chain

Resources or materials are considered 'scarce' or 'critical' when there is a high demand from industry combined with a risk of their supply. A more straightforward manner to plot the different elements is shown in Figure 2, in which the probability of a supply disturbance is plotted against the period of availability. In this graph we can distinguish three groups: critical elements, frugal elements, and elements of hope.

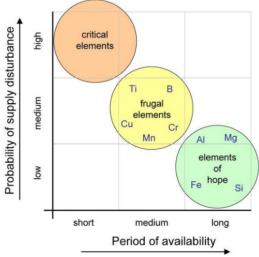


Figure 2: The three types of chemical elements [15]

The **EU criticality methodology** [16]–[18] was used to further clarify or define the critical elements for the EU states. The 2017 EU criticality assessment was carried out for 61 candidate materials (58 individual materials and 3 material groups: heavy rare earth elements, light rare earth elements, platinum group metals, amounting to 78 materials in total) [17]–[19]. This brings the number up to 27 raw materials which are now considered critical by the EU Commission (shown in Figure 3).

2017 CRMs (27)					
Antimony	Fluorspar	LREEs	Phosphorus		
Baryte	Gallium	Magnesium	Scandium		
Beryllium	Germanium	Natural graphite	Silicon metal		
Bismuth	Hafnium	Natural rubber	Tantalum		
Borate	Helium	Niobium	Tungsten		
Cobalt	HREEs	PGMs	Vanadium		
Coking coal	Indium	Phosphate rock			

Figure 3: 2017 critical raw materials list, [17]–[19]

2.1.3 Material value

The scarcity or criticality of materials is highly connected with material value or price, therefore, Prices of elements and their compounds list [20], Asian Metal market [21], and London Metal Exchange [22] prices were used to estimate the material value.

2.2 The Life Cycle Inventory Assessment of critical materials

Based on the procedure shown in Figure 1 the Life Cycle Inventory (LCI) tables for all considered FCH technologies (SOFCs, PEMFCs, PEMWEs, and AWEs) were obtained and are shown in Tables 1 - 4, respectively. Additionally, materials comprising the balance of plant (BoP) components were added to the LCI assessment and are shown in Table 5. The material is marked as critical if it is classified:

- either as hazardous,
- high in value,
- high in supply criticality and
- classified as medium in both price and supply criticality.

2.2.1 LCI table for SOFC

SOFCs materials mainly consist of rare earth elements (REE) which makes this FCH technology critical from the perspective of the EU states. Also, these materials are classified as rather costly and hazardous.



Component	Material	Material hazardousness	Material value	Supply criticality
Electrolyte	Yttria-stabilised zirconia (YSZ)	Non-hazardous	Medium	High
Electrolyte	Cerium gadolinium oxide*	Non-hazardous	Medium	High
Anode	Nickel-based oxide doped with YSZ	Hazardous (Cat. 1 carcinogen)	Medium	High
Anode	Nickel	Hazardous (Cat. 1 carcinogen)	Medium	High
Cathode	Strontium-doped lanthanum manganite	Hazardous (Irritant)	Medium	High
Callioue	Lanthanum Strontium Cobalt Ferrite*	Hazardous (Irritant)	Medium	High
	Doped lanthanum chromate	Hazardous (Irritant, harmful)	Medium	Medium-High
Interconnect	Inert metals/alloys	Non-hazardous	Medium	Medium
	Ferritic stainless steel*	Non-hazardous	Low	Low
Sealant	Glass/Glass-ceramic	Non-hazardous	Low	Low
Sedidiit	Phyllosilicates (e.g. Vermiculite, Mica)	Non-hazardous	Low	Low
Substrate	Ceramic	Non-hazardous	Low	Low

Table 1: List of common materials in SOFC [15], [16], [20], [23], [24], [22], [21]

The most critical materials are marked with red brackets.

* Materials added to the list after last Workshop in Brussels (26.9.2017).

2.2.2 LCI table for PEMFC

PEMFCs materials are mainly low-to-medium in cost with the exception of Pt or Pt-alloy catalysts. Pt and graphite, which is typically used for bipolar plates and represents a significant proportion in weight and volume of the stack, are classified as critical for the EU states. Majority of the materials used in this FCH technology are classified as non-hazardous.

Component	Material	Material hazardousness	Material value	Supply criticality
	Perfluorosulphonic acid (PFSA)	Non-hazardous	Medium	Medium
Electrolyte	Sulfonated polyether ether ketone (s-PEEK)	Non-hazardous	Medium	Low
Liectiolyte	polystyrene sulfonic acid (PSSA)	Non-hazardous	Low	Medium
	polybenzimidazole (PBI) doped with H ₃ PO ⁴ *	Hazardous (corrosive)	Medium	Low
Anode and Cathode - GDL	Carbon cloth or paper treated with hydrophobic agent	Non-hazardous	Low	Low
	Metallic mesh or cloth (e.g. stainless steel)	Non-hazardous	Low	Low
Anada and Cathoda - Catalyst layer	Platinum or Pt-alloys	Non-hazardous	High	High
Anode and Cathode - Catalyst layer	Catalyst support (carbon, metal oxides, carbides, etc.)	Non-hazardous	Medium	Low
Interconnect	Synthetic graphite or graphite composites	Non-hazardous	Low	Medium
Interconnect	Stainless steel	Non-hazardous	Low	Low
Sealant	Thermoplastic	Non-hazardous	Low	Low
Sedidit	Elastomer	Non-hazardous	Low	Low

Table 2: List of common materials in PEMFC [15], [16], [20], [23], [24], [22], [21]

The most critical materials are marked with red brackets.

* used only in high-temperature PEMFC

2.2.3 LCI table for PEMWE

PEMWEs materials are more expensive compared to the PEMFCs. The OER catalysts are based on REE while the HER catalysts are based on Pt, which means that these materials are also classified as critical and high in costs. The materials are mainly non-hazardous with the exception of the REE used for OER catalysts.

Component Material		Material hazardousness	Material value	Supply criticality
	Perfluorosulphonic acid (PFSA)	Non-hazardous	Medium	Medium
Electrolyte	Sulfonated polyether ether ketone (s-PEEK)	Non-hazardous	Medium	Low
Catalyst layer - Cathode	Pt or Pt-alloys	Non-hazardous	High	High
Cataluat Jawas Anada	Iridium and Ir-alloys Hazardous (irritant, I		High	High
Catalyst layer - Anode	Ruthenium and Ru-alloys Hazardous (toxic, carcinogen)		Medium	High
	Thermally sintered Ti	Non-hazardous	Low	Medium
Anode and Cathode -	Anode and Cathode - Ti or stainless steel mesh		Low	Medium
GDL	Synthetic graphite or graphite composites (only possible on cathode side)	Non-hazardous	Low	Medium
Interconnect	Coated titanium or Ti-alloys	Non-hazardous	Low	Medium
Sealant	Thermoplastic	Non-hazardous	Low	Low
Sedidiil	Elastomer	Non-hazardous	Low	Low

Table 3: List of common materials in PEMWE	[15], [16	6], [20]	[23]	, [24],	[22], [21]	
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The most critical materials are marked with red brackets.

2.2.4 LCI table for AWE

AWEs materials are mainly low in costs with the exception of both the anode and the cathode catalysts, which are also classified as critical for the EU states. This FCH technology is also classified as rather hazardous since the alkaline electrolyte in liquid form is used. Also, Ni-based catalyst and asbestos diaphragms, used in older types of AWEs, are classified as carcinogen.

Component	Material	Material hazardousness	Material value	Supply criticality
Electrolyte	Potassium Hydroxide	Hazardous (corrosive)	Medium	Low
Anode	Precious metals	Non-hazardous	High	High
Anode	Plastic	Non-hazardous	Low	Low
Cathada	Raney-Nickel	Hazardous (carcinogen)	Medium	High
Cathode	Plastic	Non-hazardous	Low	Low
Interconnect	Plastic	Non-hazardous	Low	Low
Sealant	Thermoplastic	Non-hazardous	Low	Low
Sealant	Elastomer	Non-hazardous	Low	Low
Diaphragm	Asbestos	Hazardous (carcinogen)	Low	Low
(membrane)	Polymers	Non-hazardous	Medium	Low

Table 4: List of common materials in AWE [24], [15], [23], [16], [20]-[22]

The most critical materials are marked with red brackets.

2.2.5 LCI table for balance of plant (BoP) components

BoP materials are more or less well defined as these devices are commonly used outside of FCH technologies. However, certain critical or at least valuable materials are also used in BoP components. Therefore, these materials and the methods to extract them should also be identified.

CO	MPONENTS	EoL waste				
BoP components	Blower or compressor	Metals, plastics				
	Humidification membrane	Metals, plastics, polymers				
	Pumps	Metals, Teflon [®] , rubbers, plastics				
	Regulators	Metals, plastics, rubbers				
	Deionising filter	Metals, plastics, resins				
	Pipes	Metals, plastics, rubbers				
	Valves	Metals, plastics, nylon, Teflon®				
	Gaskets (piping system)	Paper, plastics, rubbers				
	Thermal insulation system	Mineral wool, fibreglass				
	Heat exchangers	Metals				
	Water condensers	Stainless steel				
Ancillary BoP	PCBs	Metals, plastics, semiconductors,				
components		precious metals				
	Power conditioning system	Metals, plastics, semiconductors,				
		precious metals				
	Sensors	Plastics, precious metals,				
		semiconductors, glass				
Other	Batteries	Plastics, Lithium-ion				
components	FCH external cabinet	metal (ferrous material,				
		aluminium, steel product)				

Table 5: List of common materials in BoP

() Hy Tech Cycling

3. LCA of considered FCH materials

LCA is a methodological tool used to quantitatively analyse the life cycle of products/activities. ISO 14040 and 14044 provide a generic framework, [25], [26]. Once goal and scope of the study are determined, all relevant data are collected the scope of inventory assessment and a life cycle assessment method are defined, numerical models could be set up and a result calculated. This result is usually a very long list of emissions, consumed resources and sometimes other items. The interpretation of this list is difficult. Life cycle Impact Assessment (LCIA) procedure is designed to help with this interpretation, [8], [27].

3.1 Life Cycle Impact Assessment methodology

For the purpose of the LCA commercial software GaBi Thinkstep will be used, [28]. In GaBi Thinkstep environment all major impact assessment methodologies, such as: TRACI 2.0, CML 1996, 2001, and 2007, Eco indicator 95 and 99, Ecological Scarcity Method (UBP), EDIP, USEtox and ReCiPe, [8]. These methodologies are extensively described in Appendix of D4.1, [1]. Using these impact methodologies results can be evaluated using environmental impact indicators. In many LCA studies CML 2001 LCIA method is used, representing the midpoint approach to interpretation of the results. However, in last period ReCiPe method is used more frequently because it combines both the midpoint and the endpoint approach. As already described in D4.1, [1] the main approach will be the midpoint approach with CML2001 LCIA methodology used.

3.2 Impact indicators within CML2001 LCIA methodology

The midpoint and endpoint indicators are explained more in detail in Appendix of D4.1, [1]. The basic approach in the HyTechCycling project will be the midpoint approach (CML2001, ReCiPe). By using this approach useful information for industry sectors that deal with disassembly of systems and recycling of FCH technologies will be obtained. For CML2001 LCIA methodology main impact indicators are:

Global

- CML2001 Jan. 2016, Global Warming Potential (GWP 100 years) [kg CO2 eq.]
- CML2001 Jan. 2016, Global Warming Potential (GWP 100 years), excl biogenic carbon [kg CO2 eq.]
- CML2001 Jan. 2016, Abiotic Depletion (ADP elements) [kg Sb eq.]
- CML2001 Jan. 2016, Abiotic Depletion (ADP fossil) [MJ]
- CML2001 Jan. 2016, Ozone Layer Depletion Potential (ODP, steady state) [kg R11 eq.]

Regional

- CML2001 Jan. 2016, Acidification Potential (AP) [kg SO2 eq.]
- CML2001 Jan. 2016, Freshwater Aquatic Ecotoxicity Pot. (FAETP inf.) [kg DCB eq.]
- CML2001 Jan. 2016, Marine Aquatic Ecotoxicity Pot. (MAETP inf.) [kg DCB eq.]
- CML2001 Jan. 2016, Terrestric Ecotoxicity Potential (TETP inf.) [kg DCB eq.]

Local

- CML2001 Jan. 2016, Eutrophication Potential (EP) [kg Phosphate eq.]
- CML2001 Jan. 2016, Human Toxicity Potential (HTP inf.) [kg DCB eq.]
- CML2001 Jan. 2016, Photochem. Ozone Creation Potential (POCP) [kg Ethene eq.]



3.3 Normalization of results

To properly compare the LCA results of all the materials in the production process, from ore in the mine to the material at the FCH technology manufacturing company, they will be normalized per 1 g of mass. Further, results of each impact indicator will be normalized to the material that exhibits the lowest value. This way all the materials will be ranked proportionally to the least harmful material.

3.4 Assessment of availability of materials in LCA databases

The most commonly used materials in all the represented FCH technologies were identified in D2.1 and are shown in Section 2.1.3. To successfully execute the LCA, these materials must be available in the LCA databases or life cycle inventory has to be defined additionally. In the case of HyTechCycling project Gabi professional and Ecoinvent 3.3 databases will be used, [29], [28], [30]. If any material is missing in the database it must be replaced by a comparable material that exhibits similar properties or the material needs to be user defined. In Table 6 all the relevant and considered materials are presented and the availability in LCA libraries is identified.

3.5 Existing and novel recycling and dismantling processes

In this report the LCA study will not include the EoL phase of materials, but at least the considered materials need to be associated with possible existing or just theoretically available processes in the end of life phase of FCH technologies. The LCI database shown in Table 6 will need to be supplemented with data regarding the EoL phase of materials.

The existing EoL processes were identified in deliverable D2.2, [3], while novel EoL processes will be identified in deliverables D3.1 [4] and D3.2 [5]. The data collected in this report will be combined with data collected from those deliverables and will serve as input data for the next deliverable D4.3, where case studies with new strategies in dismantling and recycling stages will be performed.



Material	Technology	Availability in databases	EoL technologies according to D3.1 ³
Aluminium	BoP	available1	conventional
Asbestos	AWE	available1	n.r.
Carbon	PEMFC	available1	SED
Cerium gadolinium oxide	SOFC	unavailable ²	n.r.
Copper	BoP	available1	conventional
Glass-ceramic	SOFC	unavailable ²	conventional; HDT
Graphite	PEMFC	available1	n.r.
Gold	BoP	available1	HMT; PMT; novel
Iridium	PEMWE	unavailable ²	HMT; PMT
Lanthanum chromate	SOFC	purchasable1	N/A
Lanthanum Strontium Cobalt Ferrite	SOFC	unavailable ²	N/A
Lead	BoP	available1	conventional
Lithium-ion (LiFePO ₄)	BoP	available1	n.r.
Nickel	SOFC, AWE, BoP	available1	HDT; HMT
Nickel-based oxide doped with YSZ	SOFC	unavailable ²	n.r.
Palladium	SOFC, PEMFC, BoP	available1	HMT; PMT; SED; TD; AP
PEEK	AWE, PEMWE, PEMFC	purchasable1	AP; AD
PFSC (Nafion)	AWE, PEMWE, PEMFC	purchasable1	AP; AD
Phyllosilicates (Vermiculite, Mica,)	SOFC	available1	n.r.
Plastics	AWE, BoP	available1	conventional
Platinum	SOFC, PEMFC	available1	HMT; PMT; SED; TD; AP
Potassium Hydroxide	AWE	available1	n.r.
Rubber (Viton, Kalrez, Silicone,)	AWE, PEMWE, PEMFC, BoP	available1	n.r.
Ruthenium	PEMWE, PEMFC	purchasable1	HMT; PMT
Silver	SOFC, AWE, BoP	available1	HMT
Steel product	SOFC, PEMWE, PEMFC, BoP	available1	conventional
Strontium-doped lanthanum manganite	SOFC	unavailable ²	N/A
PTFE (Teflon)	AWE, PEMWE, PEMFC, BoP	purchasable1	AP; AD
Tin	BoP	available1	conventional
Titanium	PEMWE	available1	HMT
Yttria-stabilised zirconia (YSZ)	SOFC	unavailable ²	HDT

¹ available or purchasable in Ecoinvent 3.3

² unavailable in GaBi or Ecoinvent 3.3 databases

³ HDT: hydrothermal treatment; HMT: hydrometallurgical treatment; PMT: pyrometallurgical treatment; TD: transient dissolution; AP: acid process; SED: selective electrochemical dissolution; AD: alcohol dissolution; N/A: not available; n.r.: not reported





4. Results

Numerical model was set up in Gabi Thinkstep and set to 1 g of mass of specific considered material in the production phase from ore to the market. Figure 4 shows the numerical model for all identified (most common) materials used in FCH technologies modelled for manufacturing phase.

Each box represents production phase of the material up to market. Environmental impact assessments for each material are analysed with LCIA methodology CML2001- 2016 for 1 g of manufactured material for the market. All 12 midpoint environmental indicators were analysed and the LCIA results are presented, in absolute values in Table 7 and normalized to minimum value for each impact indicator (marked with red bracket) in

Table 8, for all considered materials that are available in LCA databases (till the end of December 2017). It should be noted that currently not all of the relevant materials are available in the databases (see Table 6).

In the following subsections each of the environmental indicators is shown and analysed in a separate diagram for all the materials which are present in FCH technologies and BoP components.

Hytechcycling - materials in production phase_v2

Process plan: Mass [kg] The names of the basic processes are shown

EU-28: Aluminium ingot mix ts	x <u>Im</u> ,	CA: Nafion - for use in fuel cell ts	x <u>iiii</u>
GLO: market for asbestos, crysotile type ecoinvent 3.3	х° о .	GLO: market for vermiculite ecoinvent 3.3	х°о.
GLO: market for carbon black ecoinvent 3.3	х° о .	GLO: market for polyethylene, high density, granulate	х° о .
GLO: market for copper ecoinvent 3.3	х° о .	GLO: market for platinum ecoinvent 3.3	х° о .
GLO: market for graphite ecoinvent 3.3	х°о.	GLO: market for potassium hydroxide ecoinvent 3.3	х° о .
GLO: market for gold ecoinvent 3.3	х°о.	GLO: market for silicone product ecoinvent 3.3	х° о .
EU-28: Lanthanum Chromate production (estimation) ts	x ⊕'	ZA: Ruthenium ts	x <u>k</u>
EU-28: Lanthanum Chromate production (estimation) ts GLO: market for lead ecoinvent 3.3	x⊚' x₀'	ZA: Ruthenium ts GLO: market for silver ecoinvent 3.3	x <mark>m</mark> x _° o,
GLO: market for lead ecoinvent 3.3 DE: Lithium Iron Phosphate/ Carbon Composition	x.°	GLO: market for silver ecoinvent 3.3 GLO: market for metal working, average for steel	x*o.
GLO: market for lead ecoinvent 3.3 DE: Lithium Iron Phosphate/ Carbon Composition (cathode active material) ts	x	GLO: market for silver ecoinvent 3.3 GLO: market for metal working, average for steel product manufacturing ecoinvent 3.3	x*o, X*o,

Figure 4: Numerical model in Gabi from ore to the market of considered materials



Table 7: Life cycle impact indicators for 1 g of material according to CML2001 LCIA methodology

	ADP elements [kg Sb-Eq.]	ADP fossil [MJ]	AP [kg SO2- Eq.]	EP [kg PO4-Eq.]	FAETP [kg DCB-Eq.]	GWP 100 years, [kg CO2-Eq.]	GWP 100 years, excl biogenic carbon [kg CO2-Eq.]	HTP [kg DCB-Eq.]	MAETP [kg DCB- Eq.]	ODP [kg R11-Eq.]	POCP [kg Ethene- Eq.]	TETP [kg DCB-Eq.]
Aluminium	4,30E-09	9,32E-02	4,32E-05	2,48E-06	6,04E-05	8,59E-03	8,58E-03	4,10E-02	1,99E+01	8,39E-14	2,36E-06	1,88E-05
Asbestos	1,18E-10	9,42E-04	5,56E-07	1,40E-07	1,95E-05	7,91E-05	7,88E-05	3,79E-05	7,19E-02	8,27E-12	4,22E-08	3,73E-07
Carbon black	5,02E-09	8,50E-02	1,15E-05	2,95E-06	2,12E-04	2,54E-03	2,54E-03	8,91E-04	6,86E-01	1,09E-09	8,53E-07	8,53E-06
Copper	1,81E-06	3,97E-02	3,69E-04	2,65E-04	6,76E-02	4,01E-03	4,09E-03	2,64E-01	1,91E+02	2,46E-10	1,66E-05	8,64E-04
Graphite	1,17E-10	9,15E-04	5,32E-07	1,37E-07	1,89E-05	7,55E-05	7,53E-05	3,68E-05	6,84E-02	8,35E-12	4,08E-08	3,67E-07
Gold	5,56E-02	1,87E+02	1,56E-01	1,57E+00	3,98E+02	1,59E+01	1,59E+01	5,77E+02	1,13E+06	1,62E-06	1,21E-02	1,25E+00
Lanthanum Chromate	2,20E-07	1,34E-01	7,43E-04	1,86E-04	1,14E-04	1,36E-02	1,35E-02	3,64E-03	1,39E+00	2,64E-13	4,22E-05	5,81E-05
Lead	2,85E-06	1,76E-02	4,56E-05	5,06E-07	1,10E-05	1,71E-03	1,71E-03	5,56E-04	8,16E-02	1,22E-14	2,11E-06	5,93E-06
Lithium-ion (LiFePO4)	3,80E-08	1,53E-01	4,35E-05	5,27E-06	6,51E-05	1,02E-02	1,06E-02	8,64E-04	7,62E-01	1,25E-13	3,01E-06	7,51E-05
Nickel, 99.5%	9,20E-07	1,07E-01	3,01E-03	1,11E-04	4,92E-02	1,11E-02	1,11E-02	6,24E-02	9,86E+01	6,74E-10	1,23E-04	1,60E-04
Palladium	5,37E-04	5,74E+01	1,80E+00	3,79E-02	1,68E+01	5,12E+00	5,15E+00	1,43E+01	3,37E+04	2,38E-07	7,25E-02	2,85E-02
PEEK	2,15E-08	3,42E-01	5,23E-05	4,22E-06	8,28E-05	1,74E-02	1,73E-02	6,59E-04	9,13E-01	4,32E-14	4,25E-06	1,23E-05
PFSC (Nafion)	1,31E-07	2,12E+00	4,10E-04	9,14E-05	6,18E-06	8,31E-01	8,31E-01	3,79E-05	2,19E-02	1,83E-15	9,31E-06	4,30E-07
Vermiculite	1,76E-09	2,46E-03	3,46E-06	4,32E-07	2,45E-05	1,83E-04	1,83E-04	9,40E-05	9,51E-02	2,81E-11	2,01E-07	7,13E-07
Plastics (HDPE)	2,65E-10	6,75E-02	7,09E-06	7,29E-07	8,90E-05	2,06E-03	2,05E-03	1,26E-04	4,25E-01	1,47E-11	1,41E-06	5,35E-07
Platinum	2,24E-03	3,11E+02	2,53E+00	2,69E-01	8,53E+01	2,85E+01	2,87E+01	9,30E+01	2,14E+05	8,58E-07	1,04E-01	1,39E-01
Potassium hydroxide	1,18E-08	2,34E-02	1,18E-05	4,13E-06	8,47E-04	2,13E-03	2,12E-03	1,43E-03	3,08E+00	1,39E-10	7,16E-07	1,49E-05
Silicone product	1,32E-08	4,48E-02	1,68E-05	4,75E-06	1,27E-03	3,21E-03	3,17E-03	1,60E-03	7,13E+00	1,94E-09	1,58E-06	1,10E-05
Ruthenium	3,71E-04	6,31E+01	7,86E-02	3,44E-03	5,36E-03	6,43E+00	6,43E+00	4,54E-01	6,24E+02	2,45E-10	3,70E-03	8,04E-03
Silver	5,07E-04	3,69E+00	3,25E-03	5,55E-03	1,29E+00	3,35E-01	3,41E-01	1,90E+00	3,94E+03	2,73E-08	2,58E-04	1,94E-03
Steel product	9,39E-09	2,09E-02	1,13E-05	5,14E-06	3,47E-03	2,19E-03	2,13E-03	2,84E-03	1,45E+01	1,11E-10	1,18E-06	6,00E-05
PTFE (Teflon)	1,60E-06	2,04E-01	4,06E-05	2,86E-06	3,25E-05	1,21E-02	1,21E-02	4,36E-04	7,87E-01	6,06E-10	2,97E-06	9,78E-06
Tin	1,90E-05	2,53E-01	5,15E-04	5,54E-05	7,55E-03	2,38E-02	2,38E-02	1,00E-02	2,99E+01	1,52E-09	2,59E-05	7,33E-05
Titanium	6,79E-08	3,23E-01	1,69E-04	9,10E-05	1,59E-02	3,12E-02	3,11E-02	1,63E-02	4,69E+01	3,57E-09	2,27E-05	1,13E-04



Table 8: Normalized to minimum value for each life cycle impact indicator according to CML2001 LCIA methodology

	ADP elements	ADP fossil	АР	EP	FAETP	GWP 100 years	GWP 100 years, excl biogenic carbon	НТР	МАЕТР	ODP	РОСР	ТЕТР
Aluminium	3,68E+01	1,02E+02	8,11E+01	1,81E+01	9,77E+00	1,14E+02	1,14E+02	1,11E+03	9,11E+02	4,58E+01	5,79E+01	5,13E+01
Asbestos	1,01E+00	1,03E+00	1,05E+00	1,02E+00	3,16E+00	1,05E+00	1,05E+00	1,03E+00	3,28E+00	4,52E+03	1,03E+00	1,02E+00
Carbon black	4,29E+01	9,29E+01	2,16E+01	2,15E+01	3,43E+01	3,36E+01	3,37E+01	2,42E+01	3,13E+01	5,96E+05	2,09E+01	2,32E+01
Copper	1,54E+04	4,34E+01	6,94E+02	1,94E+03	1,09E+04	5,32E+01	5,43E+01	7,17E+03	8,74E+03	1,34E+05	4,06E+02	2,35E+03
Graphite	1,00E+00	1,00E+00	1,00E+00	1,00E+00	3,06E+00	1,00E+00	1,00E+00	1,00E+00	3,12E+00	4,56E+03	1,00E+00	1,00E+00
Gold	4,75E+08	2,04E+05	2,93E+05	1,15E+07	6,44E+07	2,11E+05	2,11E+05	1,57E+07	5,16E+07	8,85E+08	2,97E+05	3,41E+06
Lanthanum Chromate	1,88E+03	1,46E+02	1,40E+03	1,36E+03	1,84E+01	1,80E+02	1,79E+02	9,89E+01	6,35E+01	1,44E+02	1,03E+03	1,58E+02
Lead	2,44E+04	1,92E+01	8,57E+01	3,69E+00	1,78E+00	2,26E+01	2,27E+01	1,51E+01	3,73E+00	6,67E+00	5,17E+01	1,62E+01
Lithium-ion (LiFePO4)	3,25E+02	1,67E+02	8,18E+01	3,85E+01	1,05E+01	1,35E+02	1,41E+02	2,35E+01	3,48E+01	6,83E+01	7,38E+01	2,05E+02
Nickel, 99.5%	7,86E+03	1,17E+02	5,66E+03	8,10E+02	7,96E+03	1,47E+02	1,47E+02	1,70E+03	4,50E+03	3,68E+05	3,01E+03	4,36E+02
Palladium	4,59E+06	6,27E+04	3,38E+06	2,77E+05	2,72E+06	6,78E+04	6,84E+04	3,89E+05	1,54E+06	1,30E+08	1,78E+06	7,77E+04
PEEK	1,84E+02	3,74E+02	9,83E+01	3,08E+01	1,34E+01	2,30E+02	2,30E+02	1,79E+01	4,17E+01	2,36E+01	1,04E+02	3,35E+01
PFSC (Nafion)	1,12E+03	2,32E+03	7,71E+02	6,67E+02	1,00E+00	1,10E+04	1,10E+04	1,03E+00	1,00E+00	1,00E+00	2,28E+02	1,17E+00
Vermiculite	1,50E+01	2,69E+00	6,50E+00	3,15E+00	3,96E+00	2,42E+00	2,43E+00	2,55E+00	4,34E+00	1,54E+04	4,93E+00	1,94E+00
Plastics (HDPE)	2,26E+00	7,38E+01	1,33E+01	5,32E+00	1,44E+01	2,73E+01	2,72E+01	3,42E+00	1,94E+01	8,03E+03	3,46E+01	1,46E+00
Platinum	1,91E+07	3,40E+05	4,76E+06	1,96E+06	1,38E+07	3,77E+05	3,81E+05	2,53E+06	9,77E+06	4,69E+08	2,55E+06	3,79E+05
Potassium hydroxide	1,01E+02	2,56E+01	2,22E+01	3,01E+01	1,37E+02	2,82E+01	2,82E+01	3,89E+01	1,41E+02	7,60E+04	1,75E+01	4,06E+01
Silicone product	1,13E+02	4,90E+01	3,16E+01	3,47E+01	2,06E+02	4,25E+01	4,21E+01	4,35E+01	3,26E+02	1,06E+06	3,87E+01	3,00E+01
Ruthenium	3,17E+06	6,90E+04	1,48E+05	2,51E+04	8,67E+02	8,52E+04	8,54E+04	1,23E+04	2,85E+04	1,34E+05	9,07E+04	2,19E+04
Silver	4,33E+06	4,03E+03	6,11E+03	4,05E+04	2,09E+05	4,44E+03	4,53E+03	5,16E+04	1,80E+05	1,49E+07	6,32E+03	5,29E+03
Steel product	8,03E+01	2,28E+01	2,12E+01	3,75E+01	5,61E+02	2,90E+01	2,83E+01	7,72E+01	6,62E+02	6,07E+04	2,89E+01	1,63E+02
PTFE (Teflon)	1,37E+04	2,23E+02	7,63E+01	2,09E+01	5,26E+00	1,60E+02	1,61E+02	1,18E+01	3,59E+01	3,31E+05	7,28E+01	2,66E+01
Tin	1,62E+05	2,77E+02	9,68E+02	4,04E+02	1,22E+03	3,15E+02	3,16E+02	2,72E+02	1,37E+03	8,31E+05	6,35E+02	2,00E+02
Titanium	5,80E+02	3,53E+02	3,18E+02	6,64E+02	2,57E+03	4,13E+02	4,13E+02	4,43E+02	2,14E+03	1,95E+06	5,56E+02	3,08E+02

In the table materials according to which results were normalized are marked with red bracket for each environmental indicator separately



4.1 Global impact indicators

• CML2001 - Jan. 2016, Global Warming Potential (GWP 100 years) [kg CO2 eq.]

The mechanism of the greenhouse effect can be observed on a small scale, as the name suggests, in a greenhouse. These effects are also occurring on a global scale. The occurring short-wave radiation from the sun comes into contact with the earth's surface and is partly absorbed (leading to direct warming) and partly reflected as infrared radiation. The reflected part is absorbed by so-called greenhouse gases in the troposphere and is re-radiated in all directions, including back to earth. In addition to the natural mechanism, the greenhouse effect is enhanced by human activates. Greenhouse gases that are considered to be caused or increased by humans are, for example: carbon dioxide, methane, CFCs. This results in a warming effect at the earth's surface. The GWP is calculated in carbon dioxide equivalents (CO2-Eq.). Figure 5 shows results and comparison for GWP of all materials considered in FCH technologies normalized per value of graphite, which is 1. For GWP per 1 g has platinum followed by gold, ruthenium and palladium.

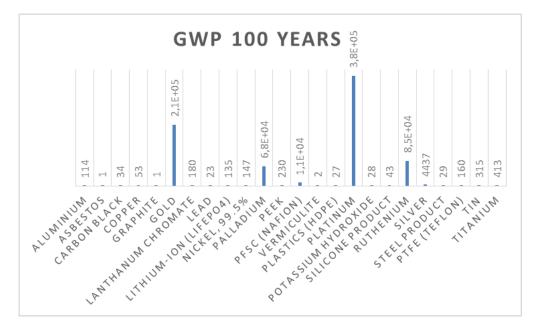


Figure 5: Normalized global warming potential for 1 gram of material

• CML2001 - Jan. 2016, Abiotic Depletion (ADP elements) [kg Sb eq.]

The abiotic depletion potential covers all natural resources (incl. fossil energy carriers) as metal containing ores, crude oil and mineral raw materials. Abiotic resources include all raw materials from non-living resources that are non-renewable. This impact category describes the reduction of the global amount of non-renewable raw materials. Non-renewable means a time frame of at least 500 years. This impact category covers an evaluation of the availability of natural elements in general, as well as the availability of fossil energy carriers. The reference substance for the characterisation factors is antimony equivalent. Figure 6 and Figure 7 shows comparison for ADP for all materials considered in FCH technologies normalized per value of graphite, which is 1. Gold is excluded from Figure 6 due to its extensively high impact. Results show that gold has the highest ADP followed by platinum, palladium, silver and ruthenium. For the ADP Fossil indicator, the highest value has platinum followed by gold, ruthenium, palladium and silver.





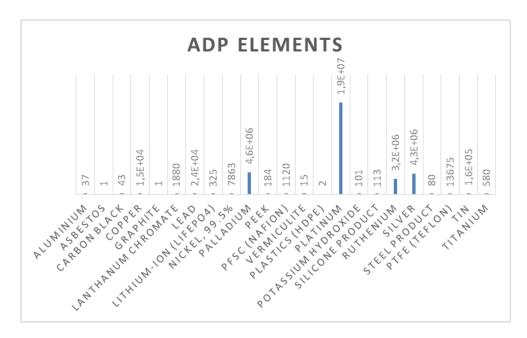


Figure 6: Normalized abiotic depletion potential (elements) for 1 gram of material (gold is excluded)

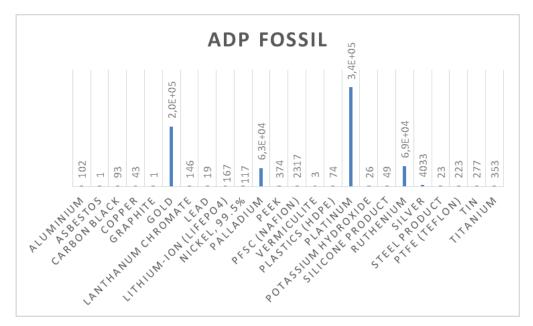


Figure 7: Normalized abiotic depletion potential (fossil) for 1 gram of material

CML2001 - Jan. 2016, Ozone Layer Depletion Potential (ODP, steady state) [kg R11 eq.]

Anthropogenic emissions deplete ozone. This is well-known from reports on the hole in the ozone layer. The substances which have a depleting effect on the ozone can essentially be divided into two groups; the fluorine-chlorine-hydrocarbons (CFCs) and the nitrogen oxides (NO_X). One effect of ozone depletion is the warming of the earth's surface. The sensitivity of humans, animals and plants to UV-B and UV-A radiation is of particular importance. Possible effects are changes in growth or a decrease in harvest crops (disruption of photosynthesis), indications of tumour's (skin cancer and eye diseases) and decrease of sea plankton, which would strongly affect the food chain. Results for ODP indicator (see Figure 8) show that



the highest value has gold (excluded in Figure 8 for better presentation) followed by Pt, Pa and Ag. All results are normalized to Nafion which has the lowest ODP indicator.

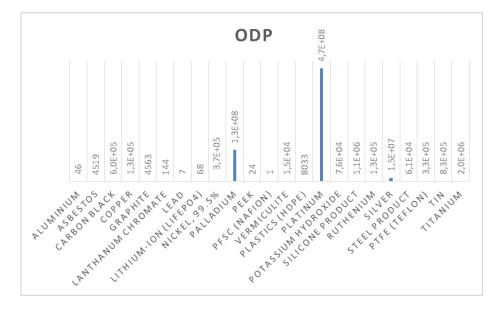


Figure 8: Normalized ozone depletion potential for 1 gram of material (gold is excluded)

4.2 Regional impact indicators

• CML2001 - Jan. 2016, Acidification Potential (AP) [kg SO2 eq.]

The acidification of soils and waters occurs predominantly through the transformation of air pollutants into acids. This leads to a decrease in the pH-value of rainwater and fog from 5.6 to 4 and below. Sulphur dioxide and nitrogen oxide and their respective acids (H₂SO₄ und HNO₃) produce relevant contributions. This damages ecosystems, whereby forest dieback is the most well-known impact. Results show that the highest AP has platinum followed by palladium, gold, ruthenium, silver and nickel. For AP the normalized values per graphite are presented in

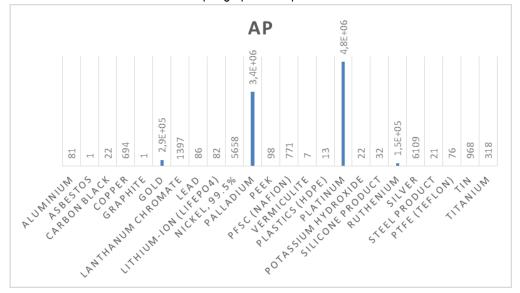


Figure 9.



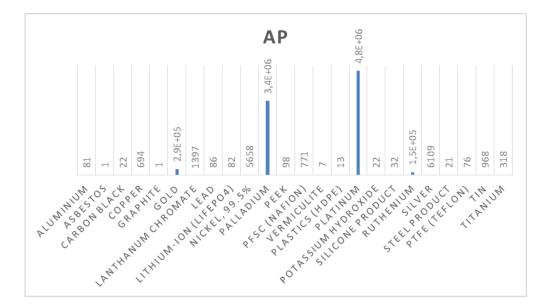


Figure 9: Normalized acidification potential for 1 gram of material

- CML2001 Jan. 2016, Freshwater Aquatic Eco-toxicity Pot. (FAETP inf.) [kg DCB eq.]
- CML2001 Jan. 2016, Marine Aquatic Eco-toxicity Pot. (MAETP inf.) [kg DCB eq.]
- CML2001 Jan. 2016, Terrestrial Eco-toxicity Potential (TETP inf.) [kg DCB eq.]

The Eco-Toxicity potential aims to outline the damaging effects on an ecosystem. This is differentiated into Terrestrial Eco-toxicity Potential (TETP), Marine Aquatic Eco-toxicity Potential (MAETP) and Freshwater Aquatic Eco-toxicity Potential (FAETP). In general, one distinguishes acute, sub-acute/sub-chronic and chronic toxicity, defined by the duration and frequency of the impact. The toxicity of a substance is based on several parameters. Therefore, the potential toxicity of a substance based on its chemical composition, physical properties, point source of emission and its behaviour and whereabouts, is characterised according to its release to the environment. Harmful substances can spread to the atmosphere, into water bodies or into the soil. Therefore, potential contributors to important toxic loads are ascertained. Detailed results for all three Eco-toxicities are presented in Table 7 and

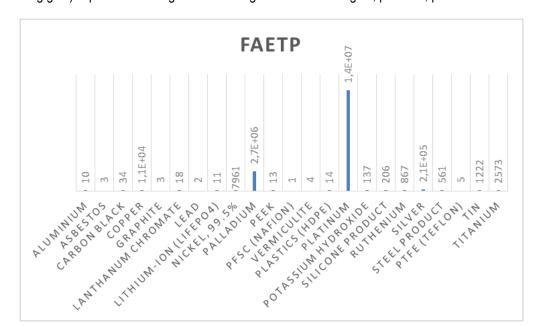


Table 8. Normalized values for these environmental indicators are similar, that is why only FAETP (excluding gold) is presented in Figure 10. The highest values have gold, platinum, palladium and silver.



Figure 10: Normalized freshwater aquatic eco-toxicity potential for 1 gram of material (gold is excluded)

4.3 Local impact indicators

• CML2001 - Jan. 2016, Eutrophication Potential (EP) [kg Phosphate eq.]

Eutrophication is the enrichment of nutrients in a certain place. Air pollutants, waste water and fertilization in agriculture all contribute to eutrophication. The result in water is an accelerated algae growth, which in turn, prevents sunlight from reaching the lower depths. This leads to a decrease in photosynthesis and less oxygen production. On eutrophicated soils, an increased susceptibility of plants to diseases and pests is often observed, as is a degradation of plant stability. If the nutrification level exceeds the amounts of nitrogen necessary for a maximum harvest, it can lead to an enrichment of nitrate. This can cause, by means of leaching, increased nitrate content in groundwater. Nitrate also ends up in drinking water. Results for EP show (gold is excluded from Figure 11) that the highest value has gold followed by platinum, palladium, silver and ruthenium.

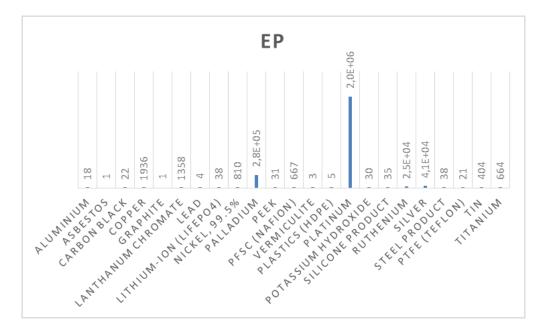


Figure 11: Normalized eutrophication potential for 1 gram of material (gold is excluded)

• CML2001 - Jan. 2016, Human Toxicity Potential (HTP) [kg DCB eq.]

The Human Toxicity Potential (HTP) assessment aims to estimate the negative impact, for example: of a process on humans. Results for HTP show (gold is excluded from Figure 12) the highest HTP value has gold followed by platinum, palladium, silver and ruthenium.



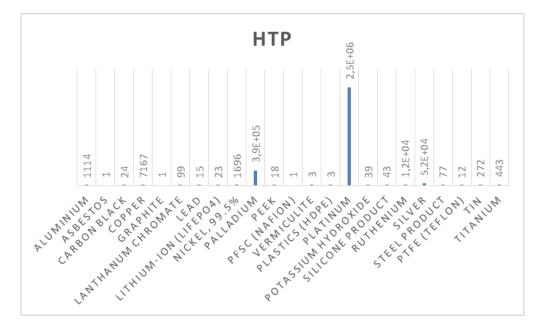


Figure 12: Normalized human toxicity potential for 1 gram of material (gold is excluded)

• CML2001 - Jan. 2016, Photochemical Ozone Creation Potential (POCP) [kg Ethene eq.]

Despite playing a protective role in the stratosphere, at ground-level ozone is classified as a damaging trace gas. Photochemical ozone production in the troposphere, also known as summer smog, is suspected to damage vegetation and material. High concentrations of ozone are toxic to humans. In Figure 13 the results for POCP are presented. The highest value of POCP has platinum followed by palladium, gold, ruthenium and silver.

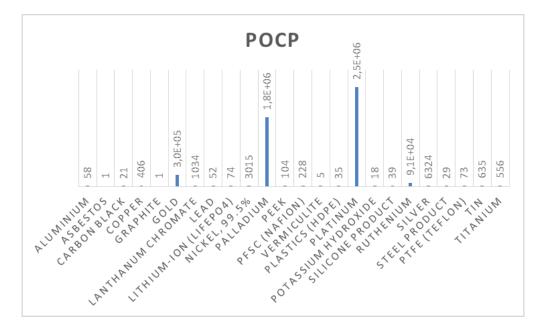




Figure 13: Normalized POC potential for 1 gram of material

4.4 Results sorted according to FCH technology under consideration and BoP

In this subsection the results of LCA are sorted according the FCH technologies under consideration. Also, the LCA results for BoP components are presented separately. This way, potentially most critical (environmentally harmful) materials can be identified within each FCH technology and BoP. For each FCH technology the most influential materials are marked with red border (three per each environmental indicator) in the tables below.

However, it needs to be pointed out that more realistic assessment will be made in the next deliverable D4.3. To adequately perform the LCA case studies, some reference FCH applications (systems) will be selected wherein actual masses of all the materials present in these systems will be taken into account.

4.4.1 <u>PEMFC</u>

All of the materials that are commonly used in PEMFCs, and are listed in Table 9, are available in the databases. This will facilitate and contribute to the accuracy of the LCA study because no substitute materials are needed.

Material	Technology	Availability in databases	EoL technologies according to D3.1 ³
Carbon	PEMFC	available1	SED
Graphite	PEMFC	available1	n.r.
Palladium	SOFC, PEMFC, BoP	available1	HMT; PMT; SED; TD; AP
PEEK	AWE, PEMWE, PEMFC	purchasable1	AP; AD
PFSC (Nafion)	AWE, PEMWE, PEMFC	purchasable ¹	AP; AD
Platinum	SOFC, PEMFC	available1	HMT; PMT; SED; TD; AP
Rubber (Viton, Kalrez, Silicone,)	AWE, PEMWE, PEMFC, BoP	available1	n.r.
Ruthenium	PEMWE, PEMFC	purchasable1	HMT; PMT
Steel product	SOFC, PEMWE, PEMFC, BoP	available1	conventional
Polytetrafluoroethylene (PTFE) -Teflon	AWE, PEMWE, PEMFC, BoP	purchasable ¹	AP; AD

Table 9: L	ist of releva	int materials f	for LCA	of PEMFC

¹ available or purchasable in Ecoinvent 3.3

² unavailable in GaBi or Ecoinvent 3.3 databases

Table 10: Normalized to minimum value for each life cycle impact indicator for PEMFC materials

³ HDT: hydrothermal treatment; HMT: hydrometallurgical treatment; PMT: pyrometallurgical treatment; TD: transient dissolution; AP: acid process; SED: selective electrochemical dissolution; AD: alcohol dissolution; N/A: not available; n.r.: not reported



	ADP elements	ADP fossil	АР	EP	FAETP	GWP	GWP, ex. biogenic carbon	НТР	MAETP	ODP	РОСР	TETP
Carbon black	4,3E+01	9,3E+01	2,2E+01	2,2E+01	3,4E+01	3,4E+01	3,4E+01	2,4E+01	3,1E+01	6,0E+05	2,1E+01	2,3E+01
Graphite	1,0E+00	1,0E+00	1,0E+00	1,0E+00	3,1E+00	1,0E+00	1,0E+00	1,0E+00	3,1E+00	4,6E+03	1,0E+00	1,0E+00
Palladium	4,6E+06	6,3E+04	3,4E+06	2,8E+05	2,7E+06	6,8E+04	6,8E+04	3,9E+05	1,5E+06	1,3E+08	1,8E+06	7,8E+04
PEEK	1,8E+02	3,7E+02	9,8E+01	3,1E+01	1,3E+01	2,3E+02	2,3E+02	1,8E+01	4,2E+01	2,4E+01	1,0E+02	3,4E+01
PFSC (Nafion)	1,1E+03	2,3E+03	7,7E+02	6,7E+02	1,0E+00	1,1E+04	1,1E+04	1,0E+00	1,0E+00	1,0E+00	2,3E+02	1,2E+00
Platinum	1,9E+07	3,4E+05	4,8E+06	2,0E+06	1,4E+07	3,8E+05	3,8E+05	2,5E+06	9,8E+06	4,7E+08	2,5E+06	3,8E+05
Silicone product	1,1E+02	4,9E+01	3,2E+01	3,5E+01	2,1E+02	4,3E+01	4,2E+01	4,3E+01	3,3E+02	1,1E+06	3,9E+01	3,0E+01
Ruthenium	3,2E+06	6,9E+04	1,5E+05	2,5E+04	8,7E+02	8,5E+04	8,5E+04	1,2E+04	2,8E+04	1,3E+05	9,1E+04	2,2E+04
Steel product	8,0E+01	2,3E+01	2,1E+01	3,8E+01	5,6E+02	2,9E+01	2,8E+01	7,7E+01	6,6E+02	6,1E+04	2,9E+01	1,6E+02
PTFE (Teflon)	1,4E+04	2,2E+02	7,6E+01	2,1E+01	5,3E+00	1,6E+02	1,6E+02	1,2E+01	3,6E+01	3,3E+05	7,3E+01	2,7E+01

In the Table 11 most environmentally influential materials are marked with red bracket

The results in Table 9 and Table 10 show that the highest environmental impacts per 1 g of material in PEMFC technology have palladium, platinum, ruthenium.

4.4.2 <u>PEMWE</u>

From the list in Table 11 it can be seen that majority of the materials that are commonly used in PEMWEs are available in the databases, the only material that is missing is iridium. However, it is expected that ruthenium is a good substitute in the LCA study because they are both platinum group metals (PGM). Hence, they have similar physical and chemical properties and also tend to occur together in the same mineral deposits.

Table 11: List of relevant materials for LCA of PEMWE										
Material	Technology	Availability in databases	EoL technologies according to D3.1 ³							
Iridium	PEMWE	unavailable ²	HMT; PMT							
PEEK	AWE, PEMWE, PEMFC	purchasable1	AP; AD							
PFSC (Nafion)	AWE, PEMWE, PEMFC	purchasable1	AP; AD							
Rubber (Viton, Kalrez, Silicone,)	AWE, PEMWE, PEMFC, BoP	available1	n.r.							
Ruthenium	PEMWE, PEMFC	purchasable1	HMT; PMT							
Steel product	SOFC, PEMWE, PEMFC, BoP	available1	conventional							
Polytetrafluoroethylene (PTFE) -Teflon	AWE, PEMWE, PEMFC, BoP	purchasable1	AP; AD							
Titanium	PEMWE	available1	НМТ							

¹ available or purchasable in Ecoinvent 3.3

² unavailable in GaBi or Ecoinvent 3.3 databases

³ HDT: hydrothermal treatment; HMT: hydrometallurgical treatment; PMT: pyrometallurgical treatment; TD:

transient dissolution; AP: acid process; SED: selective electrochemical dissolution; AD: alcohol dissolution; N/A: not available; n.r.: not reported

Table 12: Normalized to minimum value for each life cycle impact indicator for PEMWE materials



PEEK	2,3E+00	1,6E+01	4,6E+00	1,5E+00	1,3E+01	7,9E+00	8,1E+00	1,7E+01	4,2E+01	2,4E+01	3,6E+00	2,9E+01
PFSC (Nafion)	1,4E+01	1,0E+02	3,6E+01	3,2E+01	1,0E+00	3,8E+02	3,9E+02	1,0E+00	1,0E+00	1,0E+00	7,9E+00	1,0E+00
Silicone product	1,4E+00	2,1E+00	1,5E+00	1,7E+00	2,1E+02	1,5E+00	1,5E+00	4,2E+01	3,3E+02	1,1E+06	1,3E+00	2,6E+01
Ruthenium	4,0E+04	3,0E+03	7,0E+03	1,2E+03	8,7E+02	2,9E+03	3,0E+03	1,2E+04	2,8E+04	1,3E+05	3,1E+03	1,9E+04
Steel product	1,0E+00	1,0E+00	1,0E+00	1,8E+00	5,6E+02	1,0E+00	1,0E+00	7,5E+01	6,6E+02	6,1E+04	1,0E+00	1,4E+02
PTFE (Teflon)	1,7E+02	9,8E+00	3,6E+00	1,0E+00	5,3E+00	5,5E+00	5,7E+00	1,2E+01	3,6E+01	3,3E+05	2,5E+00	2,3E+01
Titanium	7,2E+00	1,5E+01	1,5E+01	3,2E+01	2,6E+03	1,4E+01	1,5E+01	4,3E+02	2,1E+03	2,0E+06	1,9E+01	2,6E+02

In the Table 12 most environmentally influential materials are marked with red bracket

The Table 9: List of relevant materials for LCA of PEMFCresults in Table 11 and Table 12 show that the highest environmental impacts per 1 g of material in PEMWE technology have ruthenium, titanium, Nafion and PTFE (Teflon).

4.4.3 <u>AWE</u>

All of the materials that are commonly used in AWEs, and are listed in Table 13, are available in the databases. This will facilitate and contribute to the accuracy of the LCA study because no substitute materials are needed.

Material	Technology	Availability in databases	EoL technologies according to D3.1 ³
Asbestos	AWE	available1	n.r.
Nickel	SOFC, AWE, BoP	available1	HDT; HMT
PEEK	AWE, PEMWE, PEMFC	purchasable1	AP; AD
PFSC (Nafion)	AWE, PEMWE, PEMFC	purchasable1	AP; AD
Plastics	AWE, BoP	available1	conventional
Potassium Hydroxide	AWE	available1	n.r.
Rubber (Viton, Kalrez, Silicone,)	AWE, PEMWE, PEMFC, BoP	available1	n.r.
Silver	SOFC, AWE, BoP	available1	HMT
Polytetrafluoroethylene (PTFE) -Teflon	AWE, PEMWE, PEMFC, BoP	purchasable1	AP; AD

 Table 13: List of relevant materials for LCA of AWE

¹ available or purchasable in Ecoinvent 3.3

² unavailable in GaBi or Ecoinvent 3.3 databases

³ HDT: hydrothermal treatment; HMT: hydrometallurgical treatment; PMT: pyrometallurgical treatment; TD: transient dissolution; AP: acid process; SED: selective electrochemical dissolution; AD: alcohol dissolution; N/A: not available; n.r.: not reported



	ADP elements	ADP fossil	АР	EP	FAETP	GWP	GWP, ex. biogenic carbon	НТР	MAETP	ODP	РОСР	ТЕТР
Asbestos	1,0E+00	1,0E+00	1,0E+00	1,0E+00	3,2E+00	1,0E+00	1,0E+00	1,0E+00	3,3E+00	4,5E+03	1,0E+00	1,0E+00
Nickel, 99.5%	7,8E+03	1,1E+02	5,4E+03	7,9E+02	8,0E+03	1,4E+02	1,4E+02	1,6E+03	4,5E+03	3,7E+05	2,9E+03	4,3E+02
PEEK	1,8E+02	3,6E+02	9,4E+01	3,0E+01	1,3E+01	2,2E+02	2,2E+02	1,7E+01	4,2E+01	2,4E+01	1,0E+02	3,3E+01
PFSC (Nafion)	1,1E+03	2,3E+03	7,4E+02	6,5E+02	1,0E+00	1,1E+04	1,1E+04	1,0E+00	1,0E+00	1,0E+00	2,2E+02	1,2E+00
Plastics (HDPE)	2,2E+00	7,2E+01	1,3E+01	5,2E+00	1,4E+01	2,6E+01	2,6E+01	3,3E+00	1,9E+01	8,0E+03	3,3E+01	1,4E+00
Potassium hydroxide	1,0E+02	2,5E+01	2,1E+01	3,0E+01	1,4E+02	2,7E+01	2,7E+01	3,8E+01	1,4E+02	7,6E+04	1,7E+01	4,0E+01
Silicone product	1,1E+02	4,8E+01	3,0E+01	3,4E+01	2,1E+02	4,1E+01	4,0E+01	4,2E+01	3,3E+02	1,1E+06	3,7E+01	2,9E+01
Silver	4,3E+06	3,9E+03	5,8E+03	4,0E+04	2,1E+05	4,2E+03	4,3E+03	5,0E+04	1,8E+05	1,5E+07	6,1E+03	5,2E+03
PTFE (Teflon)	1,4E+04	2,2E+02	7,3E+01	2,0E+01	5,3E+00	1,5E+02	1,5E+02	1,2E+01	3,6E+01	3,3E+05	7,0E+01	2,6E+01

Table 14: Normalized to minimum value for each life cycle impact indicator for AWE materials

In the table 3 most environmentally influential materials are marked with red bracket

The results in Table 13 and Table 14 Table 9: List of relevant materials for LCA of PEMFCshow that the highest environmental impacts per 1 g of material in AWE technology have silver, nickel, and Nafion followed by silicon product and Teflon.

4.4.4 <u>SOFC</u>

As can be seen from Table 15 many materials that are commonly used in SOFCs are missing in the databases. This means that the results may be somewhat distorted because the materials that are missing might have considerable impact on the environment. Unfortunately, it is also rather difficult to find substitute materials since these materials are specific cermets (ceramic-metal composites).



Material	Technology	Availability in databases	EoL technologies according to D3.1 ³
Cerium gadolinium oxide	SOFC	unavailable ²	n.r.
Glass-ceramic	SOFC	unavailable ²	conventional; HDT
Lanthanum chromate	SOFC	purchasable1	N/A
Lanthanum Strontium Cobalt Ferrite	SOFC	unavailable ²	N/A
Nickel	SOFC, AWE, BoP	available1	HDT; HMT
Nickel-based oxide doped with YSZ	SOFC	unavailable ²	n.r.
Palladium	SOFC, PEMFC, BoP	available1	HMT; PMT; SED; TD; AP
Phyllosilicates (Vermiculite, Mica,)	SOFC	available1	n.r.
Platinum	SOFC, PEMFC	available1	HMT; PMT; SED; TD; AP
Silver	SOFC, AWE, BoP	available1	HMT
Steel product	SOFC, PEMWE, PEMFC, BoP	available1	conventional
Strontium-doped lanthanum manganite	SOFC	unavailable ²	N/A
Yttria-stabilised zirconia (YSZ)	SOFC	unavailable ²	HDT

Table 15: List of relevant materials for LCA of SOFC

¹ available or purchasable in Ecoinvent 3.3

 $^{\rm 2}$ unavailable in GaBi or Ecoinvent 3.3 databases

³ HDT: hydrothermal treatment; HMT: hydrometallurgical treatment; PMT: pyrometallurgical treatment; TD: transient dissolution; AP: acid process; SED: selective electrochemical dissolution; AD: alcohol dissolution; N/A: not available; n.r.: not reported

	ADP elements	ADP fossil	AP	EP	FAETP	GWP	GWP, ex. biogenic carbon	НТР	MAETP	ODP	РОСР	TETP
Lanthanum Chromate	1,3E+02	5,4E+01	2,1E+02	4,3E+02	4,7E+00	7,4E+01	7,4E+01	3,9E+01	1,5E+01	1,0E+00	2,1E+02	8,1E+01
Nickel, 99.5%	5,2E+02	4,3E+01	8,7E+02	2,6E+02	2,0E+03	6,1E+01	6,1E+01	6,6E+02	1,0E+03	2,6E+03	6,1E+02	2,2E+02
Palladium	3,1E+05	2,3E+04	5,2E+05	8,8E+04	6,9E+05	2,8E+04	2,8E+04	1,5E+05	3,5E+05	9,0E+05	3,6E+05	4,0E+04
Vermiculite	1,0E+00	1,0E+00	1,0E+00	1,0E+00	1,0E+00	1,0E+00	1,0E+00	1,0E+00	1,0E+00	1,1E+02	1,0E+00	1,0E+00
Platinum	1,3E+06	1,3E+05	7,3E+05	6,2E+05	3,5E+06	1,6E+05	1,6E+05	9,9E+05	2,3E+06	3,3E+06	5,2E+05	1,9E+05
Silver	2,9E+05	1,5E+03	9,4E+02	1,3E+04	5,3E+04	1,8E+03	1,9E+03	2,0E+04	4,1E+04	1,0E+05	1,3E+03	2,7E+03
Steel product	5,3E+00	8,5E+00	3,3E+00	1,2E+01	1,4E+02	1,2E+01	1,2E+01	3,0E+01	1,5E+02	4,2E+02	5,9E+00	8,4E+01

Table 16: Normalized to minimum value for each life cycle impact indicator for SOFC materials

In the table 3 most environmentally influential materials are marked with red bracket

The results in Table 15 and Table 16 Table 9: List of relevant materials for LCA of PEMFCshow that the highest environmental impacts per 1 g of material in SOFC FCH technologies have palladium, platinum and silver. These results are inconclusive; due to unavailable LCI data in databases for 6 commonly used materials in SOFC technologies. There is communication with GaBi software developers whether the missing data could be obtained.

4.4.5 <u>BoP</u>

Since BoP components are commonly used outside of FCH technologies the materials that comprise them (see Table 17) are more or less well supported in the databases, therefore, no substitute materials are needed.



Material	Technology	Availability in databases	EoL technologies according to D3.1 ³		
Aluminium	BoP	available ¹	conventional		
Copper	BoP	available1	conventional		
Gold	BoP	available1	HMT; PMT; novel		
Lead	BoP	available1	conventional		
Lithium-ion (LiFePO ₄)	BoP	available1	n.r.		
Nickel	SOFC, AWE, BoP	available1	HDT; HMT		
Palladium	SOFC, PEMFC, BoP	available1	HMT; PMT; SED; TD; AP		
Plastics	AWE, BoP	available1	conventional		
Rubber (Viton, Kalrez, Silicone,)	AWE, PEMWE, PEMFC, BoP	available1	n.r.		
Silver	SOFC, AWE, BoP	available1	HMT		
Steel product	SOFC, PEMWE, PEMFC, BoP	available1	conventional		
Polytetrafluoroethylene (PTFE) -Teflon	AWE, PEMWE, PEMFC, BoP	purchasable1	AP; AD		
Tin	BoP	available1	conventional		

¹ available or purchasable in Ecoinvent 3.3

² unavailable in GaBi or Ecoinvent 3.3 databases

³ HDT: hydrothermal treatment; HMT: hydrometallurgical treatment; PMT: pyrometallurgical treatment; TD: transient dissolution; AP: acid process; SED: selective electrochemical dissolution; AD: alcohol dissolution; N/A: not available; n.r.: not reported

Table 18: Normalized to minimum value for each life cycle impact indicator for BoP materials

	ADP elements	ADP	АР	EP	FAETP	GWP	GWP, ex. biogenic	НТР	MAETP	ODP	РОСР	TETP
	elements	fossil					carbon					
Aluminium	1,6E+01	5,3E+00	6,1E+00	4,9E+00	5,5E+00	5,0E+00	5,0E+00	3,3E+02	2,4E+02	6,9E+00	2,0E+00	3,5E+01
Copper	6,8E+03	2,3E+00	5,2E+01	5,2E+02	6,1E+03	2,3E+00	2,4E+00	2,1E+03	2,3E+03	2,0E+04	1,4E+01	1,6E+03
Gold	2,1E+08	1,1E+04	2,2E+04	3,1E+06	3,6E+07	9,3E+03	9,3E+03	4,6E+06	1,4E+07	1,3E+08	1,0E+04	2,3E+06
Lead (99,995%)	1,1E+04	1,0E+00	6,4E+00	1,0E+00	1,0E+00	1,0E+00	1,0E+00	4,4E+00	1,0E+00	1,0E+00	1,8E+00	1,1E+01
LiFePO4	1,4E+02	8,7E+00	6,1E+00	1,0E+01	5,9E+00	6,0E+00	6,2E+00	6,9E+00	9,3E+00	1,0E+01	2,6E+00	1,4E+02
Nickel, 99.5%	3,5E+03	6,1E+00	4,2E+02	2,2E+02	4,5E+03	6,5E+00	6,5E+00	5,0E+02	1,2E+03	5,5E+04	1,0E+02	3,0E+02
Palladium	2,0E+06	3,3E+03	2,5E+05	7,5E+04	1,5E+06	3,0E+03	3,0E+03	1,1E+05	4,1E+05	2,0E+07	6,1E+04	5,3E+04
Plastics (HDPE)	1,0E+00	3,8E+00	1,0E+00	1,4E+00	8,1E+00	1,2E+00	1,2E+00	1,0E+00	5,2E+00	1,2E+03	1,2E+00	1,0E+00
Silicone product	5,0E+01	2,5E+00	2,4E+00	9,4E+00	1,2E+02	1,9E+00	1,9E+00	1,3E+01	8,7E+01	1,6E+05	1,3E+00	2,1E+01
Silver	1,9E+06	2,1E+02	4,6E+02	1,1E+04	1,2E+05	2,0E+02	2,0E+02	1,5E+04	4,8E+04	2,2E+06	2,2E+02	3,6E+03
Steel product	3,5E+01	1,2E+00	1,6E+00	1,0E+01	3,2E+02	1,3E+00	1,2E+00	2,3E+01	1,8E+02	9,1E+03	1,0E+00	1,1E+02
PTFE (Teflon)	6,0E+03	1,2E+01	5,7E+00	5,7E+00	3,0E+00	7,1E+00	7,1E+00	3,5E+00	9,6E+00	5,0E+04	2,5E+00	1,8E+01
Tin	7,2E+04	1,4E+01	7,3E+01	1,1E+02	6,9E+02	1,4E+01	1,4E+01	7,9E+01	3,7E+02	1,2E+05	2,2E+01	1,4E+02

In the table 3 most environmentally influential materials are marked with red bracket

The results in Table 17 and Table 18 Table 9: List of relevant materials for LCA of PEMFCshow that the highest environmental impacts per 1 g of material in BoP have gold followed by palladium, silver, tin and copper.



5. Conclusions

The scope of this document is to assess materials used in considered FCH technologies from environmental point of view. Materials that are most commonly present in these technologies were identified and listed. Materials used in BoP components were added to this list because they can also consist of certain critical or at least valuable materials. To identify potentially most critical (environmentally harmful) materials the LCA study was performed using Thinkstep Gabi software with Gabi professional database and Ecoinvent 3.3 database. Materials that are available in these databases were evaluated per 1 gram of material in the production stage and for interpretation of the results the LCIA midpoint CML2001 methodology was used. It should be noted that currently not all of the relevant materials are available in the databases.

The results of the LCA study show that among the listed materials the biggest impact on the environmental indicators has gold which is closely followed by other noble metals (platinum, palladium, ruthenium, and silver). This result might be slightly misleading since there are some materials missing in the LCI databases. These are mainly cermets based on REE which are present in SOFC technology. In the following LCA studies performed within the next deliverable 4.3, where case studies of reference FCH systems will be performed according to actual masses of the materials present in these systems, it is also expected that gold will have minor impact since it is only present in small amounts in the BoP components.

Further, potentially most critical (environmentally harmful) materials were identified within each FCH technology and BoP:

- The highest environmental impacts per 1 g of material in PEMFC technology have palladium, platinum, ruthenium.
- The highest environmental impacts per 1 g of material in PEMWE technology have ruthenium, titanium, Nafion and PTFE (Teflon).
- The highest environmental impacts per 1 g of material in AWE technology have silver, nickel, and Nafion followed by silicon and Teflon.
- The highest environmental impacts per 1 g of material in SOFC technology have palladium, platinum and silver. However, these results are inconclusive due to unavailable LCI data in databases for 6 commonly used materials in SOFC technologies. There is communication with GaBi software developers whether the missing data could be obtained.
- The highest environmental impacts per 1 g of material in BoP have gold followed by palladium, silver, tin and copper.





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