HYDROGEN SUPPLY AND TRANSPORTATION USING LIQUID ORGANIC HYDROGEN CARRIERS (HYSTOC)

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WP8 - Business Development and LCA

D8.1

Potential environmental implications of LOHC concepts

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Document Type	
PRO	Technical/economic progress report (internal work package reports indicating work status)
DEL	Technical reports identified as deliverables in the Description of Work
MoM	Minutes of Meeting
MAN	Procedures and user manuals
WOR	Working document, issued as preparatory documents to a Technical report
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Abbreviations

ADP	Abiotic depletion potential
ADP-E	Abiotic depletion potential of elements
ADP-FF	Abiotic depletion potential of fossil fuels
AP	Acidification potential
BOM	Bill of Materials
CO2	Carbon dioxide
CO2 eq.	Carbon dioxide equivalent
DBT	Dibenzyltoluene
EP	Eutrophication potential
GWP	Global warming potential
H2	Hydrogen
HySTOC	Hydrogen supply and transportation using liquid organic hydrogen carriers - EU-project
LCA	Life Cycle Assessment
LOHC	Liquid Organic Hydrogen Carrier
LOHC-D	Liquid Organic Hydrogen Carrier in dehydrogenated form
LOHC-H	Liquid Organic Hydrogen Carrier in hydrogenated form
POCP	Photochemical ozone creation potential
PO4--- eq.	Phosphate ion equivalent
PSA	Pressure Swing Absorption
SO2	Sulphur dioxide

1 Introduction

Hydrogen (H2) can be seen as one way to tackle climate change as a carbon free fuel. It doesn't release greenhouse gases in the use stage, but the production, storage and transportation of H2 require energy and are thus not carbon neutral. HySTOC (Hydrogen Supply and Transportation using liquid Organic hydrogen Carriers) project studies the concept of liquid organic hydrogen carrier (LOHC) used in the transportation of H2, and this deliverable is the first part of the environmental impact assessment of the concept. One of the main benefits of the LOHC concept is that the risks related to "free hydrogen" (e.g. risk of explosion/fire) are eliminated when H2 is bound to LOHC. Also, the amount of H2 transported per m3 of LOHC is higher compared to common transports using compressed gaseous hydrogen.

This environmental assessment will be split into two parts: 1) A preliminary screening and 2) a final report at the end of the HySTOC project. This report presents the intermediate results of the preliminary screening. The purpose of the preliminary screening is to identify those hot spots of the value chain that create high environmental burdens as well as those having potential to minimize impacts. This feedback can then be utilized during the later concept and system development in the project.

In this screening phase, the value chain of hydrogen transportation is modeled starting from the hydrogenation of the liquid organic carrier that is dibenzyltoluene in this project, followed by transportation, dehydrogenation and finally hydrogen purification, after which H2 would be ready to be used as a fuel. The infrastructure related to LOHC operations is also included in the study. Later on in the project the second phase of the environmental impact assessment will be made, where the concept of LOHC will be compared to traditional transportation concepts of H2, namely compressed gas and liquefied H2 transportation.

2 Life cycle assessment (LCA) methodology in HySTOC project

2.1 Life cycle assessment as a method

Environmental impact assessment is done with life cycle assessment (LCA) in this project. LCA is a standardized method (ISO 14040-44) which is commonly used to assess environmental performance of products and services. LCA consists of four stages, starting from the goal and scope definition, continuing with inventory calculation with data collection, followed by impact assessment and finally interpretation of the results. The idea is to consider the entire life cycle of a product, from material and energy production, manufacturing of the product and use stage until the final disposal or recycling, including the transportations in all relevant stages as well. However, the system boundaries can be shortened in some cases e.g. from cradle to mill gate. Each process within the life cycle is connected to the previous and next ones with material or energy flows and the chain is mathematically calculated as a balance calculation. All resources used and emissions produced during the life cycle are converted into several environmental impacts using emission specific impact assessment factors, e.g. climate change or water eutrophication, and calculated per a specific unit describing the need that is fulfilled with the product or service, called the functional unit.

In addition to the ISO standards on LCA, there are public guidance documents called FC-Hy Guides for performing LCAs on fuel cells (Masoni and Zamagni, 2011) and hydrogen production technologies (Lozanovski et al. 2011). These documents are particularly aimed for projects funded by the Fuel Cells and Hydrogen Joint Undertaking (FCH JU), giving technical guidance on functional units, system boundaries, allocation rules, and other relevant issues. This study follows the main principals of both ISO standards and FC-Hy Guides.

2.2 LCA in HySTOC

Lozanovski et al. (2011) state that the hydrogen delivery chain LCA should use a cradle-to-gate boundary, meaning that the production of hydrogen with purification and conditioning is mandatory, while the distribution of H2 is optional. The use phase would cause equal amount of emissions in all hydrogen use cases and is therefore excluded from the study. However, also H2 production was decided to be left out of this screening study, since the goal was to focus on the HySTOC concept only. Since the transportation of H2 is the key topic of HySTOC project, it is naturally included in this study. The main idea the LOHC concept in HySTOC is presented in Figure 1.

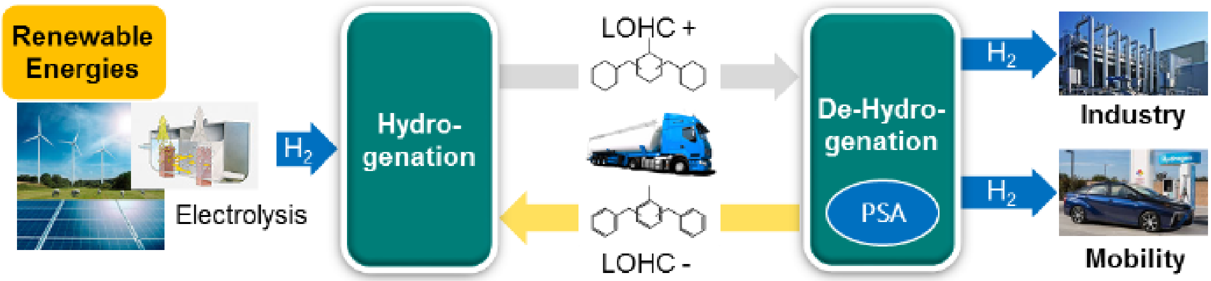

Figure 1. The main idea of HySTOC concept.

The environmental impact categories studied in this screening stage are presented in Table 1. These impact categories are calculated with CML 2001 characterization factors (CML-IA, 2018).

Table 1. Impact categories used in the study.

Impact category	Abbreviation in the reporting	Reporting unit
Global warming potential in 100 year perspective	GWP	kg CO2 equivalents
Abiotic depletion potential of elements	ADP-E	kg antimony equivalents
Abiotic depletion potential of fossil fuels	ADP-FF	MJ
Acidification potential	AP	kg SO2 equivalents
Eutrophication potential	EP	kg PO4- equivalents
Photochemical ozone creation potential	POCP	kg ethylene equivalents

3 Description of the study

3.1 The HySTOC concept for LOHC infrastructure

The life cycle boundaries of the assessment in HySTOC considers mainly the transportation of hydrogen stored in a liquid organic hydrogen carrier (LOHC) that is dibenzyltoluene (DBT). The system is presented in detail in HySTOC Deliverable 2.1 Requirement Specifications for LOHC Infrastructure (HySTOC 2018). The LCA calculations start from hydrogen being bound to DBT in a Storage Plant forming the hydrogenated form of LOHC (LOHC-H), which can bind 57 kg hydrogen / m3 LOHC-H. LOHC-H is transported to the hydrogen refuelling station, where the hydrogen is released from LOHC-H in a Release Plant and purified with a PSA Unit. The system also considers the back haul transportation of dehydrogenated DBT (LOHC-D) and regeneration of DBT after 750 cycles. The functional unit for the calculation is 1kg of transported hydrogen.

The equipment tested in the HySTOC project is only on pilot scale, but for the LCA the used equipment was scaled to represent industrial scale. This means that the Storage Plant capacity would be 10 t hydrogen / day, and the Release Plant and PSA Unit capacity would be 1 t / day. One Storage Plant would thus serve hydrogen for ten Release Plants and use locations. The expected bill of materials and the corresponding manufacturing of the equipment is included in the LCA calculation.

3.2 Data collection

The data collection for the LCA calculations was divided between project partners as presented in Table 2. This division assured that the data was as specific as possible for this project.

Table 2. Data collection between the project partners.

Life cycle stage	Partner responsible for data collection
Hydrogenation, process and Storage plant equipment	Hydrogenious
LOHC transportation	Hydrogenious
Dehydrogenation, process and Release plant equipment	Hydrogenious
PSA Unit for hydrogen purification	HyGear

The life cycle inventory data for the materials used was collected by VTT from the Ecoinvent 3.4. database with system model “Allocation at the point of substitution”. The LCI datasets used are presented in Table 3.

Table 3. The LCI datasets used in the LCA of the LOHC concept.

Material / item in the flowsheet	Name of the LCI dataset(s) from Ecoinvent 3.4	Time representativeness of the dataset
Activated carbon	Market for activated carbon, granular	2005-2017
Aluminium oxide	Market for aluminium oxide	2011-2017
Aluminium	Market for aluminium, primary, ingot Market for sheet rolling, aluminium	2010-2017 2011-2017
Cast iron	Market for cast iron	2011-2017
Chlorine	Market for chlorine, liquid	2000-2017
Copper	Market for copper Market for sheet rolling, copper	2011-2017 2011-2017
Electricity	Market group for electricity, medium voltage (Europe without Switzerland)	2014-2017
Epoxy	Market for epoxy resin	2015-2020
District heat	Market for heat, district or industrial, natural gas (Europe)	2011-2017
Nitrogen	Market for nitrogen, liquid (Europe)	2011-2017
Noble metal	Market for platinum	2012-2017
Oil	Market for lubricating oil	2011-2017
Plastic	Market for polypropylene, granulate	2011-2017
PTFE	Market for tetrafluoroethylene	2011-2017
Stainless steel	Market for steel, chromium steel 18/8, hot rolled Market for sheet rolling, chromium steel	2011-2017 2011-2017
Steel	Market for steel, low-alloyed, hot rolled Market for zinc coat, coils	2011-2017 2011-2017
Stone wool	Market for stone wool, packed	2011-2017
Toluene	Market for toluene, liquid	2011-2017
Transport	Market for transport, freight, lorry >32 metric ton, EURO6	2009-2017

3.3 Modelling and assumptions of the life cycle

The LCA calculation was done with an LCA calculation tool called SULCA 5.0. The flowsheet of the system is shown in Figure 2. The production of hydrogen, use stage of hydrogen and the end of life stage of the equipment were not considered since they are not in the scope of the study.

The transportation was modelled to take place with a 32t truck with assumed distance of 300km. The density of LOHC-H is considered to be 921kg/m3 and of LOHC-D 1016kg/m3 (Safety Data Sheet, 2016a and 2016b).

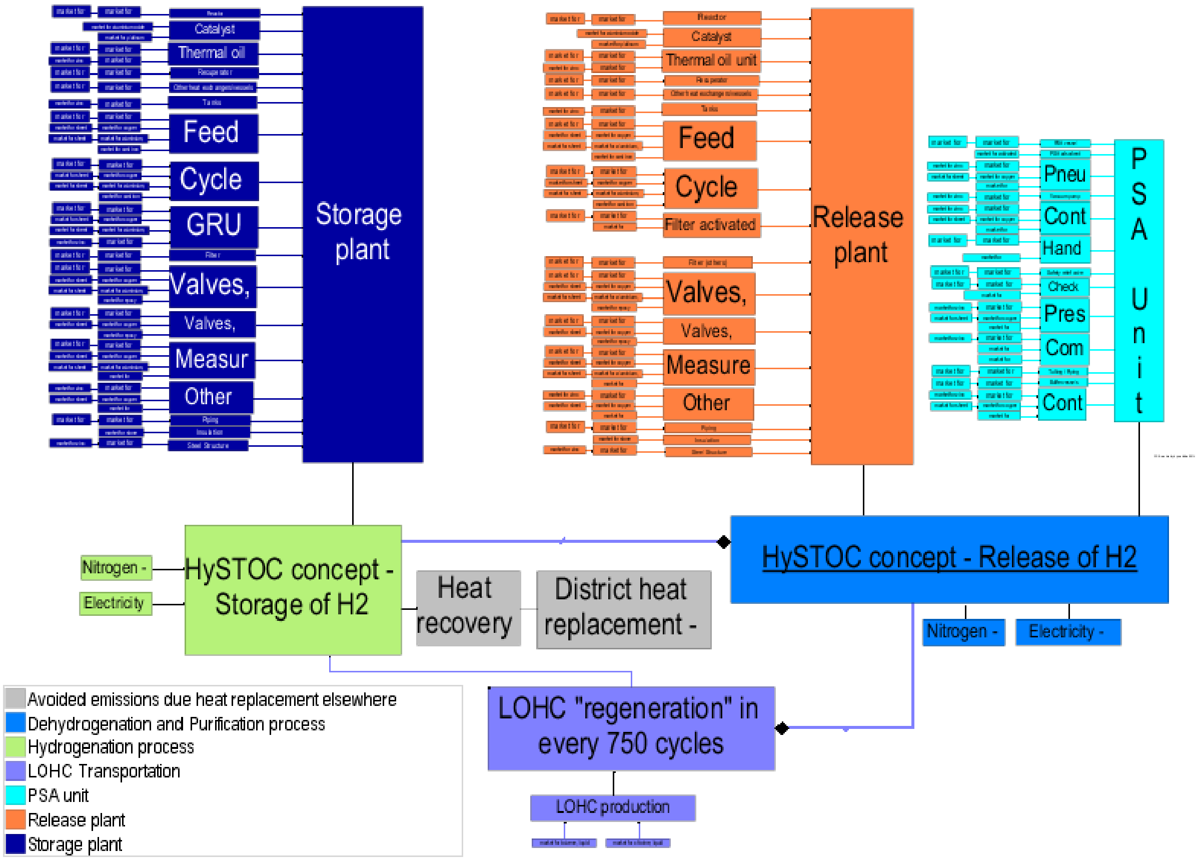

Figure 2. The flowsheet of the HySTOC concept.

Since the HySTOC system is still in the pilot scale and the industrial scale was considered for this calculation, the assumptions may have significant influence to the results and can create uncertainties that will be further elaborated in the final LCA study. The most important assumptions are listed in Table 4.

Table 4. Main assumptions used in the study and their explanation and reasoning.

Topic of assumption	Explanation / Reasoning
Size of the Storage plant	10 000 kg H2 /day. Industrial scale estimated.
Size of the Release plant	1000 kg H2 /day. Industrial scale estimated.
Size of the PSA Unit	1000 kg H2 /day. Industrial scale estimated.
Usage time of the equipment	160 000 h.
Transportation distance and vehicle	300km in a > 32 metric ton lorry (tank truck). No separate containers for LOHC needed during transportation.
Manufacturing and regeneration of dibenzyltoluene	Not included due to lack of data.

Electricity mix in use stage of Release plant and Storage plant	European average mix: 0,4546 kg CO2 e / kWh.
Energy consumption of the hydrogenation process (Storage plant)	Electricity consumption should be 90 kWh/h power at the highest.
Excess heat from the Storage plant	Due to the exothermic reaction, about 3800kW heat release is expected, with assumed 10% loss without further use. I.e. 3400kW can be useable in some other external process.
Excess heat replacing heat from natural gas.	Natural gas based heat was chosen to represent the heating option in Europe.
Energy consumption of the dehydrogenation process (Release plant + PSA unit + H2 compressor)	Assumed 530-600 kW consumption, 600 kW used in the calculations, which equals to 14,4 kWh/ kg H2. 460kW (11 kWh/kg H2) are considered as demand for reaction enthalpy. In this screening LCA, all energy consumed is assumed to be electricity.
PSA efficiency	99% efficiency used in the calculation.
H2 binding efficiency to LOHC	99,9% efficiency assumed. The 0,1% loss is expected due to physical solving and degassing.
Excess heat from the Release plant	No usable heat to other processes can be expected.
LOHC production	Dibenzyltoluene is made of toluene and chlorine. Unfortunately, no further information on the production was available so it was not considered in the study at this point. Also the regeneration after 750 cycles was not included due to lack of data.
LOHC properties	Density of LOHC-D 1016 kg/m3. Density of LOHC-H 921 kg/m3. Binding ability 57kg hydrogen / m3 LOHC-H.

4 Results of the LCA calculation

4.1 Results of the HySTOC concept without the excess heat consideration

The results of the LCA calculation for HySTOC concept per 1 kg hydrogen transported and released are presented in Figure 3. At his stage of the project only the relative impact of each process step is illustrated. The absolute values will be published in the final LCA at the end of the project. The results are reported according to the life cycle stages described earlier. The shares from each life cycle stage clearly show that the main source of all impacts is the dehydrogenation process, which creates 55-95% of emissions in all impact classes because of the high electricity demand in the process. The second important source of impacts is the LOHC transportation, causing 2-31% of emissions depending on the impact category. It is also visible that the manufacturing of the plant equipment (Storage plant, Release plant and PSA unit) has only small impact in all categories.

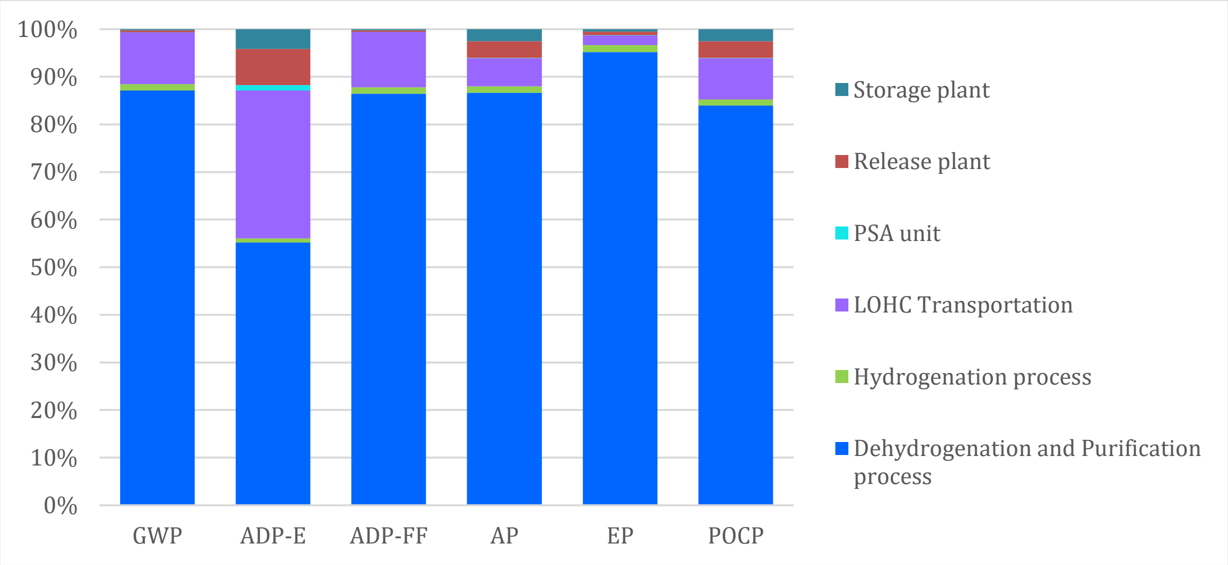

Figure 3. Shares from each life cycle stage on different impact categories without avoided emissions.

4.2 Results of the HySTOC concept with excess heat consideration

Since the hydrogenation process creates heat due to its exothermic reaction, the released heat can be exploited in some other product system. The heat can replace e.g. district heating in some locations and the emissions from the heat production would thus be avoided. This can be considered in the results by expanding the study to include also the heat production and use. Per 1 kg of transported and released hydrogen, 30MJ heat can be recovered and used elsewhere. The relative amount of avoided emissions from 30MJ natural gas based heat are presented in Figure 4. It can be seen that savings can be achieved especially in the categories of climate change (GWP) and depletion of fossil fuel resources (ADP-FF).

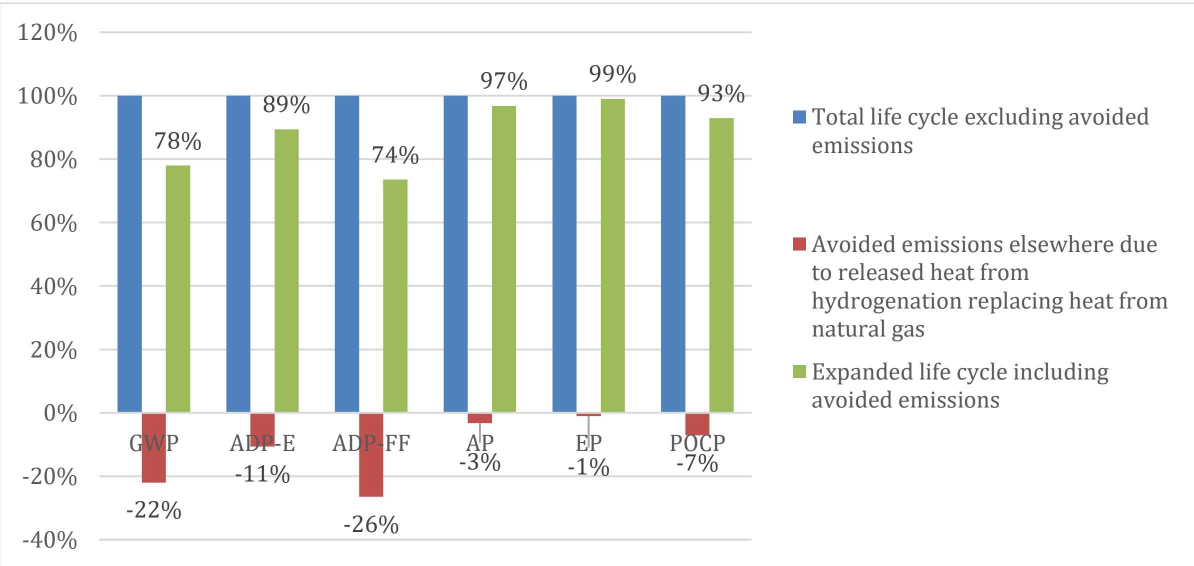

Figure 4. The impact of avoided emissions in the studied impact categories.

5 Conclusions and recommendations

The main source of impacts of HySTOC concept in all studied categories was the dehydrogenation process, causing 55-90% of all emissions. The energy demand (c.14,4 kWh / kg H2 released) of this process is a significant contributor to the overall emissions. The energy consumption of roughly 11 kWh/kg H2 for the endothermic process cannot be changed remarkably, but the energy source can. In this screening phase of LCA, all energy used in the dehydrogenation process was assumed to be electric. Therefore, the electricity source itself has a big impact on the results. To reduce the overall emissions from production and along the distribution chain, an increasing share of renewable power should be targeted to reduce the CO2 emissions per kg H2 at every step in the supply chain. Another potential lever to reduce the CO2 emissions is to replace electrical heating with a different heating source, such as natural gas or bio methane. Electricity production efficiency is typically lower than the efficiency of heat production, so the change to direct heat production instead of heating with electric power could mean significant fuel savings and thus reduced emissions. Both aspects mentioned above should be assessed in the second part of the LCA and results will be reported at the end of the HySTOC project.

It would be very beneficiary to use the excess heat from the hydrogenation process in some other system. The amount of released heat, 30 MJ / 1 kg H2 should not be lost but utilised e.g. to heat up buildings. The replaced heat could alternatively be produced from different fuels, which would affect the amount of avoided emissions and thus the total impact of the HySTOC concept. This could also be tested later on in the project.

Transportation is highly interesting in the next stage of the project when LOHC technology is compared to compressed gaseous H2 and liquefied H2. The different transportation capacities per truck must be considered, together with the back-haulage of hydrogen cylinders or LOHC. At this stage, the results show that the impact of transportation varies from 2% in eutrophication potential to 31% in abiotic depletion of elements. In climate change category, the impact from transportation is 11%. The impact of transportation distance can also be studied further in the next stage of the project, e.g. a distance of break-even point between the different methods can be calculated.

The role of H2 production was not included in the study at this point. Depending on the production method and electricity used, the carbon footprint of H2 production could vary between c. 2-30 kg CO2e/kg H2, so it could be the main contributor of greenhouse gases in the value chain. H2 production will stay the same in all alternative transportation methods, though, so it is not the most interesting source of impacts in that sense. Emissions of H2 production directly relate to the emissions from electricity production. If the production of H2 would be based on renewable energy, the emissions would be minimized. H2 production should be considered in the next stage of the LCA later on in the project.

As expected, the manufacturing of the equipment (storage plant, release plant and PSA unit) does not have a great impact on any impact category. The biggest impact is in the abiotic depletion of elementary resources, c.13 % altogether. Typically, the machinery and infrastructure can be left out of the LCA, when industrial scale production is considered. This calculation also showed that this approach is justified and that the infrastructure can be left out in the next stage of LCA.

The production and regeneration of LOHC was not included in this study due to a lack of data. It has, most likely, only a small impact in the overall results since the dibenzyltoluene can be reused up to 750 times and regenerated to a high degree afterwards. Nevertheless, the production and regeneration should be considered in the next stage of the LCA.

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