



WATER PROOF

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urban WASTE and water Treatment Emission Reduction by utilizing CO₂ for the PROduction Of Formate derived chemicals

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| ☒ R | Document report | ☒ PU | Public, fully open, e.g. web |
| ☐ DEM | Demonstrator, pilot, prototype | ☐ SEN | Sensitive, restricted under conditions set out in Model Grant Agreement |
| ☐ DEC | Websites, patent filings, videos, etc. | ☐ CI | Classified, information as referred to in Commission Decision 1001/844/EC |
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Publishable executive summary

In the WaterProof project, a TRL-6 demonstration plant is built to demonstrate the on-site conversion of CO₂ emissions captured from consumer waste incineration and wastewater treatment facilities into formic acid. This deliverable report describes the potential environmental impacts of the production of formic acid using the WaterProof demonstration plant. The functional unit has been defined as 1 kg 30wt% formic acid. The environmental impacts have been analysed throughout a cradle-to-gate system by means of Life Cycle Assessment (LCA) using the impact assessment method EF 3.1 recommended by the European Environmental Footprint initiative (EC 2022). The data for this assessment was provided by HVC and Avantium as well as Ecoinvent database 3.9 datasets were used when no primary data was available. The analysis focusses on the most relevant impact categories which have been evaluated after applying normalised and weighted factors, which help to put absolute figures into context. Based on normalised and weighted results, climate change, resource use of fossil fuels, and resource use of minerals and metals were identified as the most relevant impact categories. Additionally, particulate matter pollutants and eutrophication (freshwater) were also recognized as significant contributors within the studied product system. The analysis was done based on characterised results and the contribution analysis for these relevant impact categories.

The hotspot analysis revealed that potassium hydroxide (KOH) production, which is used in the first production step (UO1), is a major contributor to environmental impacts across various categories. Specifically, the majority of impacts originate from the upstream of KOH production namely energy and steam supply for potassium chloride production, highlighting KOH as a significant environmental hotspot. Comparisons between scenarios with renewable energy versus those with European grid mix electricity demonstrated significant differences in environmental impacts, emphasizing the importance of renewable energy sources in mitigating environmental burdens.

This LCA provides valuable insights into the environmental performance of the WaterProof process. Key findings include the dominance of climate change, resource use of fossil fuels, and resource use of minerals and metals as significant impact categories. Additionally, the hotspot analysis underscores the importance of efficient KOH utilisation to minimise environmental impacts. Benchmarking against fossil-based formic acid highlights the potential benefits of the WaterProof process, when powered by renewable energy.

Moving forward, it is essential to consider technical, economic, and social aspects alongside environmental factors for a comprehensive sustainability assessment. Continuous refinement of the LCA models and data collection will allow for a more accurate evaluation

of the WaterProof process's environmental performance as the project progresses. The information in this document will be used as a basis for the detailed and final report on LCA and S-LCA (D4.8). It should be noted that the results are only preliminary and the comparison with the benchmark only serves as an initial assessment. According to ISO 14040/14044, a correct comparison must be reviewed critically.

1 Introduction

The WaterProof project aims to close the carbon loop in waste(water) by developing an innovative biorefinery concept that converts CO₂ emissions from urban wastewater treatment facilities into valuable green consumer products. The objective is to create a technology that results in greenhouse gas reduction through CO₂ utilization, the substitution of fossil feedstocks, and the electrification of industrial processes.

Part of this project is the assessment of the environmental impacts that occur along the value chain of three final formic acid-based products (Cleaning Products, Leather Tanning and Acidic Deep Eutectic Solvents (ADES)) in cradle-to-grave assessments. Furthermore, they will also be compared to potential conventional counterparts. This analysis will be carried out by means of Life Cycle Analysis (LCA), following the well-established LCA standards laid out in ISO 14040 (ISO2006a) and ISO 14044(ISO2006b). However, this intermediate report focuses solely on the preliminary LCA of the production of formic acid in a cradle-to-gate approach, as the final products have not yet been produced at this stage of the research. Understanding the environmental impacts of the WaterProof process will be essential to further guide the process development. A full-fledged LCA to validate the potential environmental benefits, that the project is about to achieve (D4.8) will complement this initial screening and is due at the end of the project (M48).

As a consequence, the focus of this deliverable is on: 1) identifying environmental hotspots of the research project in order to guide the optimisation of the process engineering carried out in T2.2 and; 2) evaluating different electricity scenarios to provide a comprehensive picture of ecological sustainability aspects; 3) benchmarking against conventional formic acid to provide a preliminary insight regarding WaterProof formic acid overall environmental preferability.

The results of this preliminary LCA will therefore function as a reference point for environmentally comparing the WaterProof formic acid product with conventional formic acid derived from fossil sources. This analysis will aid in comprehending the advantages and/or limitations of the product developed so far.

It must also be noted, that LCA is a methodology based on several choices and many scenarios are possible (e.g., different energy supply options, different methodological options, etc.). For this initial LCA a baseline scenario was defined as a starting point of the evaluation. The findings and interpretation of the results will help identify meaningful

scenarios worth a closer look. Relevant scenarios will be discussed and evaluated within this report. These will also be included and further developed in a more detailed deliverable (D4.8) due at the end of the project.

Summing up, this report aims principally at:

- 1) identifying environmental hotspots in order to guide the process design optimisation;
- 2) evaluating various electricity scenarios to provide a comprehensive picture of ecological sustainability aspects;
- 3) benchmarking against conventional fossil-based formic acid to gain an initial insight into the environmental preferability of the WaterProof process.

The following chapters describe the environmental assessments conducted as part of WP4 and are structured as follows:

Chapter 2 The Life Cycle Assessment framework;

Chapter 3 Goal and Scope definition;

Chapter 4 Life Cycle Inventory Analysis;

Chapter 5 Life Cycle Impact Assessment;

Chapter 6 Conclusion and Outlook.

In the annex, tables with supporting information can be found.

Note that in this report, points are used as decimal separators.

2 Life Cycle Assessment framework

Life Cycle Assessment (LCA) is an internationally standardized method laid out in ISO 14040:2006 and ISO 14044:2006 to quantitatively assess the potential environmental impact of a product or service throughout its entire life cycle by quantifying all inputs and outputs of material and energy flows and assessing how these flows affect the environment (Figure 1). It assesses potential environmental impacts such as climate change, depletion of natural resources and human and ecotoxicity.

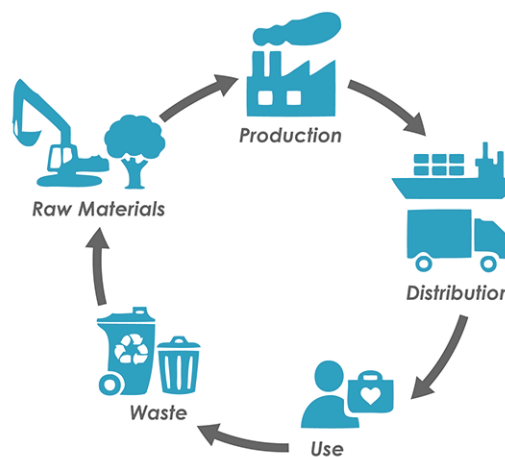


Figure 1: Life cycle of a product

An LCA study consists of four different phases:

1. Goal and scope definition
2. Life Cycle Inventory analysis (LCI)
3. Life Cycle Impact Assessment (LCIA)
4. Interpretation of the results

In the goal and scope definition phase, the product to be studied and the purpose of the study are decided on. The functional unit for which the study refers is also defined. Many other choices related to the modelling are made during the goal and scope definition (see Chapter 3).

In the life cycle inventory analysis (LCI) phase, the system model is built according to the requirements of the goal and scope definition. The system model is a flow model of the system with certain types of system boundaries. The result is a mass and energy balance for the system. In this phase the quality of the data, assumptions and limitations are also described.

The Life Cycle Impact Assessment (LCIA) aims to indicate the potential impacts of the environmental loads quantified in the inventory analysis by classifying the inventory

parameters to the type of environmental impact that they contribute to and finally by calculating the relative contribution of the emissions and resources consumption to each type of environmental impact (characterisation). Such calculations are based on scientific models of cause-effect chains in the natural system. Sometimes these results need to be interpreted and aggregated even further. This can be done in different ways, for instance by normalisation and weighting procedures.

The last phase is the interpretation in which the findings of both, the inventory analysis and the impact assessment are evaluated, in relation to the defined goal and scope, in order to reach conclusions and recommendations. The relationships between these phases have been illustrated in Figure 2 which shows that an LCA study is a highly iterative process among the different phases.

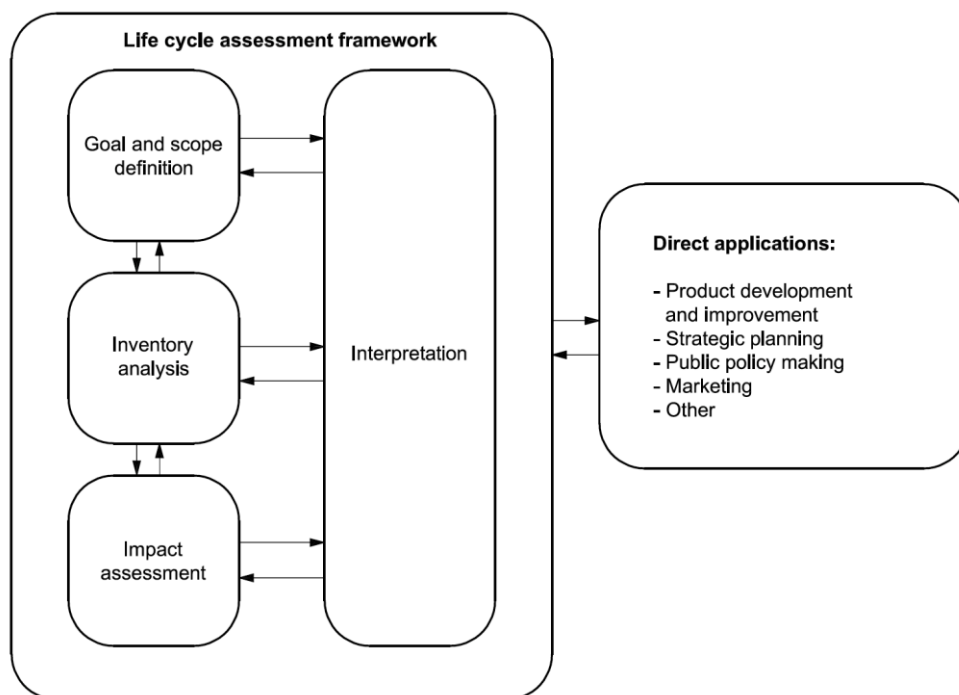


Figure 2: Life cycle assessment framework (ISO 14040)

The results of an LCA can be used for revealing hotspots which can lead to identification of approaches to mitigate the impacts for the development of less harmful processes and products (product and process design and decision making). The LCA may also enable the comparison of different products (benchmarking) and can support marketing and public policies, for instance, to support LCA-based eco-labelling. Another important application of LCA is that of learning, e.g., exploring the environmental properties of the product system studied and learning about relationships of the production system.

A final word: it is crucial to emphasize that "positive" Life Cycle Assessment (LCA) results do not automatically indicate the sustainability of a process. One limitation of the LCA is its focus solely on quantifying the ecological aspect of sustainability, thereby excluding economic and social indicators from the assessment. To obtain a comprehensive understanding of the sustainability of a process, it is imperative to also consider economic and social aspects. Therefore, a Techno-Economic Evaluation (TEE) and a Social Life Cycle Assessment (S-LCA) are conducted in T4.4 (D4.6) and T4.1 (D4.8).

3 Goal and Scope

This section provides a detailed description of the LCA methodology utilised for the study: the goal of the LCA, functional unit and reference flow, the system boundaries, the choices for the modelling approach for addressing multi-functionality, the modelling tools, data requirements, impact assessment method, assumptions and limitations.

3.1 Goal

The goal of the following preliminary LCA is to support the WaterProof research project by assessing the potential environmental impacts of the processes developed in WP1 and WP2 of the WaterProof project. The assessment focuses particularly on:

- identifying the potential environmental hotspots, allowing for the optimisation of the process throughout the course of the research project;
- evaluating different allocation scenarios to provide a comprehensive picture of ecological sustainability aspects;
- providing a comparison against conventional petrochemical formic acid.

3.2 Scope

The LCA will be conducted under an attributional approach, i.e., based on inventory of the emissions and removals from the processes used in the life cycle of the production of formic acid.

3.2.1 Targeted audience

The results of this intermediate report on environmental impacts are publicly available. However, the results are only preliminary and the comparison with the benchmark only serves as an initial assessment. According to ISO 14040/14044, a correct comparison must be reviewed critically.

3.2.2 Geographical and time and technological representativeness

The WaterProof demo plant is set to be situated at Waternet Wastewater Treatment Plant (WWTP) in Amsterdam (NL) and HVC in Alkmaar (NL). The objective of the study is to reflect the European situation of the production of WaterProof formic acid products. Therefore, corresponding background data, including all materials and utilities are considered from datasets of production in Europe (RER) whenever available.

Primary data reflects the current status (at half-way of the project) of the process design for the WaterProof processes and partly on calculations based on the maximum capacity of a process unit. As such, this is a preliminary assessment which will be updated and completed at the end of the project (D4.8).

3.2.3 Functional unit

The role of the functional unit definition in LCA is to ensure that the environmental assessment of products is based on a fair comparison. The WaterProof process yields 25wt% formic acid in water. A concentration of at least 30wt% is required for use in cleaning agents and for fish leather tanning. The formic acid must therefore be concentrated after the WaterProof process, e.g. by distillation.

The functional unit was defined as follows:

- How much: 1 kg of formic acid
- Quality: 30wt% in water
- Where: manufactured in the Netherlands (Alkmaar and Amsterdam)
- Function: Can be directly utilized or will undergo further concentration

Table 1: Physical-chemical characteristics of formic acid

Product	Formic acid (WaterProof)
Formula	CH ₂ O ₂
Molar mass	46.025 g/mol
CAS number	64-18-6
Boiling Point	100.8 °C
Bio-based carbon content	100%

3.2.4 System boundaries

Figure 3 depicts the WaterProof system boundaries. At the current stage of the project and in this deliverable (D4.1) the assessment covers the processes from cradle-to-gate. This starts with the capture and liquefaction of CO₂ at Waternet's biogas plant in Amsterdam or at HVC's CO₂ capture installation in Alkmaar. The CO₂ will be converted to formic acid (HCOOH) in three main unit operations (UO1, UO2 and UO3) as it was described in deliverable D2.1 (Engineering specifications; internal report).

The material, utilities, waste streams and direct emissions have been considered. Infrastructure or labour activities, other than those considered in background processes were not included since these data are not available and based on experience their impacts tend to be negligible compared to those arisen from materials and utilities. Long-term emissions were also excluded.

In the second half of the project the formic acid will be tested in three applications (cleaning agent, fish leather tanning and acidic deep eutectic solvent (ADES). Thus, the assessment from cradle-to-grave will be further analysed in the full-fledged LCA report in M48 (D4.8).

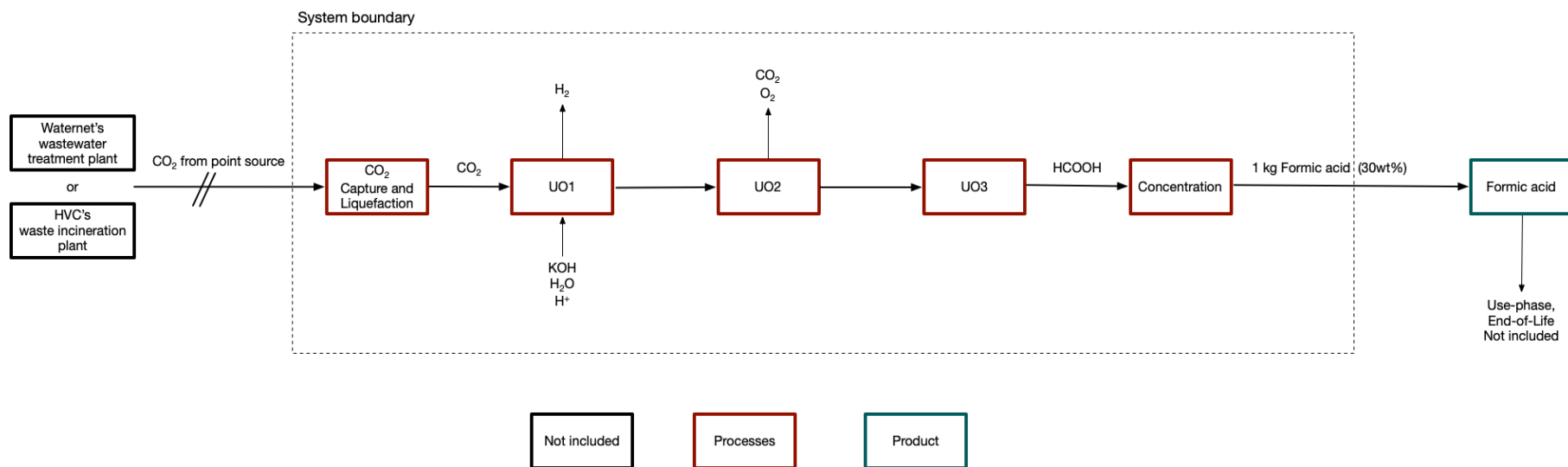


Figure 3: System boundaries of Waterproof processes

3.2.5 Allocation

In attributional LCA partitioning the input or output flows of a process (allocation) is often needed when multiple products are produced throughout the product system. In the context of this LCA allocation rules have been applied in the following situations:

- CO₂ capture & liquefaction: The capture and liquefaction of CO₂ is neither Waternet's nor HVC's main activity. However, both companies have other activities related to environmental burdens. A cut-off approach has been chosen, meaning that the other activities of both companies are not within the system boundaries of this LCA study, but that the burden of the CO₂ capture and liquefaction are 100% allocated to the CO₂ production.
- Intermediate- and co-product production: During the first (UO1) and second (UO2) process step several products are formed. The burdens were 100% allocated to the main intermediate product which leads in UO3 to the final product: formic acid.
- O₂ and H₂O: On the anode side of the UO2 only O₂ is emitted, the H₂O output drag is recirculating. Thus, the burdens were 100% allocated to O₂ production.

3.2.6 Impact categories and impact assessment method

The SimaPro 9.5 LCA software was used to model the product system and to derive environmental impacts in this study. In addition, the inventory data related to the product system included in this study were linked to the environmental impacts shown in Table 2 through the Environmental Footprint (EF) 3.1 method (EF 2022). This is the most up-to-date impact assessment method developed by the European Environmental Footprint initiative (EC 2012). EF 3.1 contains environmental characterisation factors, derived from scientifically robust and internationally recognized impact models, and assesses a complete set of indicators addressing impacts on ecosystems, human health and depletion of resources. These indicators are midpoint impacts that focus on single environmental problems. It must be noted that they represent impact potentials and do not predict impacts at endpoint level, exceeding of thresholds, safety margins or risks.

Normalised and weighted results were included in order to put absolute figures into context and allow the results among different impacts to be compared. To that aim, the normalisation and weighting factors recommended in the used EF 3.1 method (EC 2022) were applied. On this basis, the top five impact categories are analysed in this report.

In this initial LCA, and as considered in the EF 3.1 method, characterisation factors of 0 are applied for biogenic carbon uptake and release (0/0 approach), aiming to achieve zero net emissions from the biogenic carbon cycle.

Table 2: Impact categories evaluated

Impact category	Indicator	Unit
Climate change	Radiative forcing as Global Warming Potential with a time horizon of 100 years (GWP100)	kg CO ₂ eq.
Resource use, fossils	Abiotic resource depletion – fossil fuels	MJ
Resource use, minerals and metals	Abiotic resource depletion ultimate reserves	kg Sb eq
Particulate matter	Disease incidence due to exposure to PM	Disease incidence
Ozone depletion	Ozone Depletion Potential	kg CFC-11 eq.
Photochemical ozone formation	Tropospheric ozone concentration increase	kg NMVOC eq.
Ionising radiation	Human exposure efficiency relative to U ²³⁵	kBq U-235 eq.
Acidification	Accumulated Exceedance	mol N eq.
Eutrophication, freshwater	Fraction of nutrients reaching freshwater end compartment (P)	kg P eq.
Eutrophication, marine	Fraction of nutrients reaching marine end compartment (N)	kg N eq.
Eutrophication, terrestrial	Accumulated Exceedance	mol N eq.
Land use	Soil quality index ¹	Pt
Water use	User deprivation potential	m ³ deprivation
Human toxicity, non-cancer	Comparative Toxic Unit for humans	CTUh
Human toxicity, cancer	Comparative Toxic Unit for humans	CTUh
Ecotoxicity, freshwater	Comparative Toxic Unit for ecosystems	CTUe

¹ The result of the aggregation of 4 indicators provided by LANCA model (Beck et al., 2010 and Bos et al., 2016), i.e. biotic production, erosion resistance, mechanical filtration and groundwater replenishment. Indicators expressed in kg biotic production, soil or water/m² and year, aggregated as production per year and m² units (Pt).

4 Life Cycle Inventory Analysis

The Life Cycle Inventory (LCI) consists of detailed tracking of all flows that go in and out of the product system, including raw resources or materials, energy by type, water, and emissions to air, water and land by a specific substance. Inputs and outputs of all necessary processes were collected during the data collection phase. An important part of an LCA case study report is to state data sources, data gaps, taken assumptions and identified limitations that have to be considered when interpreting and concluding the results.

4.1 Data sources

The foreground data for the production of Waterproof's formic acid was provided by Avantium, Waternet and HVC. For the background processes (e.g., feedstocks, materials, and utilities) data was used from the Ecoinvent LCI inventory database (version 3.9). This database is internationally recognized, both from a qualitative (completeness of data, quality of validation process) as well as from a quantitative perspective (scope of included processes). Background production data from Ecoinvent were kept as local (Europe, RER) as possible. A table of relevant background datasets can be found in Annex A.

When necessary to fill data gaps, approximations based on expert estimations were considered. Furthermore, it is known that the LCI varies on different databases due to location, technologies, emission level, etc. The comparison of LCI from different databases is out of the scope of this study.

4.2 Assumptions

The following general assumptions at inventory level were made in order to perform LCA:

- The biogenic content of CO₂ at HVC is 98,2% and at Waternet 100%, so that CO₂ is considered 100% biogenic in this assessment. Within this study biogenic carbon uptake as well as release are considered with characterisation for uptake and release of 0 (0/0 approach).
- Electricity is supplied by high voltage renewable wind power (NL).
- Sulfuric acid used in the WaterProof process is excluded from the inventory as it was used only in catalytic amounts in UO1 (<1%) and recirculates in UO3. Thus, it can be deemed negligible.

4.3 Inventory data formic acid production

The WaterProof demonstrator will convert captured and liquefied CO₂ stemming from wastewater treatment or waste incineration to formic acid (HCOOH) using electrochemical processes. The WaterProof process consists of three steps (UO1, UO2, and UO3) which

leads to a low concentrated formic acid. Modelling a concentration step was necessary to concentrate the formic acid to 30 wt%, enabling its use for the application. Calculations were conducted to determine the energy needed to remove water from the formic acid, with an assumed efficiency of 80%. The inventory data is presented in Table 3. Since this is a public report, the quantities of the various in-and outputs are not disclosed.

Table 3: Inventory data for the production of formic acid.

In/output
Inputs from technosphere: Materials
CO ₂
KOH
H ₂ O
Inputs from technosphere: Utilities
Electricity
Products
HCOOH
O ₂
Emissions to air
H ₂
CO ₂

4.4 Data quality assessment, uncertainty analysis and limitations

Since LCA is a tool founded on quantification, uncertainty is present at the data inventory level. Incorrect estimations or modelling assumptions, outdated data and data gaps are sources of uncertainty. To validate the LCIA results discussed in Chapter 5, uncertainties and data quality in terms of representativeness and appropriateness have to be depicted as the basis for the interpretation of the results. A qualitative analysis of the uncertainty due to the variability of the inventory data is carried out (Table 4). Indications on the quality of data include the evaluation of the source, reliability, completeness and relevance (based on the environmental hotspots analysis) of the data itself, combined with the

evaluation of the representativeness (temporal, geographical and technological) of the data used to model the different product systems.

In general, the data used was rated as good in the context of the project. However, in this context, the following limitations and main sources of uncertainties were identified in this study:

- Early-stage assessment: this LCA represents processes under development (research phase). As such, early stage life cycle inventory data and environmental evaluations are associated with uncertainty, which should decrease throughout the project. In contrast, petrochemical-based formic acid is already commercially established and manufactured on optimised basis. Comparisons to the benchmark must be considered under this limitation.
- Uncertainties in foreground processes: The data for UO3 is derived from the maximum capacity of the unit. Therefore, the results of this study are valid only within the context of this assumption.
- Uncertainties in background data: Secondary data was obtained from the Ecoinvent LCA database and efforts were made to use the best available background datasets. Overall, the selection of datasets was rated as good. However, uncertainties cannot be completely excluded.

Table 4 contains the data sources for each process or material as well as an evaluation of the quality of the data in the context of the LCA.

Table 4: Data quality assessment

Process/material	Source	Quality	Comment/Dataset
CO ₂ production	Primary (HVC)	good	
KOH supply	Ecoinvent 3.9	good	Potassium hydroxide {RER} potassium hydroxide production Cut-off, U
H ₂ O supply	Ecoinvent 3.9	good	Water, deionised {Europe without Switzerland} market for water, deionised Cut-off, U
UO1 data	Primary (AVT)	good	
UO2 data	Primary (AVT)	good	
UO3 data	Primary (AVT)	adequate	
Electricity	Ecoinvent 3.9	good	Electricity, high voltage {NL} electricity production, wind, 1-3MW turbine, offshore Cut-off, U

5 Life Cycle Impact Assessment and Interpretation

This section aims at evaluating and understanding the magnitude and significance of the potential environmental impacts for the product system defined in this study.

5.1 Identification of the most relevant impact categories

LCAs generate a broad range of impact results, of which units and absolute figures are not intuitively comparable or understood by most readers. Normalisation and weighting steps can help put absolute figures into context and allow the results of different impact categories to be compared in order to assess their relative importance. Towards that aim, Table 5 shows the average relevance of the impact categories associated with the studied processes after normalising and weighting. These results were obtained using the normalisation and weighting factors recommended in the EF 3.1 method (EC 2022). The relevance of the impact category is expressed as the percentage of its contribution with respect to an overall environmental single-score considering all evaluated impacts. The exclusion of ecotoxicity from the assessment despite its contribution of over 35% is attributed to the lack of robustness in this impact category within the methodology. Consequently, while ecotoxicity may play a significant role in environmental impacts, its exclusion aims to ensure the integrity and reliability of the assessment by prioritising impact categories with higher robustness and certainty in their evaluation. Human toxicity (both cancer and non-cancer) is excluded from the assessment for similar reasons, as its robustness within the methodology is deemed inadequate.

Based on the normalised and weighted results, climate change, resource use of fossil fuels and Resource use of minerals and metals were found to be predominately the most relevant impact categories. The first two are in line with the most relevant impact categories in the current political agenda, driving the transition from fossil to renewable carbon. In addition, and to a lesser extent, particulate matter pollutants and eutrophication (freshwater) were also identified as relevant categories (>4.9% contribution) within the product system under study.

The discussion and interpretation of the results will focus on these identified top-five impact categories.

Table 5: Relevance of the EF 3.1 impact categories

Impact category	Relevance
Ecotoxicity, freshwater	32.5%
Climate change	17.2%
Resource use, fossils	12.9%
Resource use, minerals and metals	10.8%
Particulate matter	6.0%
Eutrophication, freshwater	4.9%
Acidification	3.6%
Photochemical ozone formation	2.7%
Water use	2,7%
Human toxicity, non-cancer	1,6%
Ionising radiation	1.6%
Eutrophication, terrestrial	1.4%
Eutrophication, marine	1.0%
Human toxicity, cancer	0.7%
Land use	0.5%
Ozone depletion	0.0%

5.2 Hotspot analysis

The contribution of the various components across the value chain to the identified key impact categories for the baseline scenario is further illustrated in Figure 4.

The breakdown of components includes:

- CO₂ production: this group refers to the capture and liquefaction of CO₂ which consists exclusively of energy and 100% bio-based CO₂ inputs.
- Electricity UO1+2: this group refers to the electrical use required for UO1 and UO2.
- Electricity UO3: this group refers to the electrical use required for UO3.

- Concentration: this group refers to the electrical use required for distillation
- UO1+2 excl. electricity: this group includes all emissions from UO1 and UO2 caused by every input but electricity (mainly KOH).
- UO3 excl. electricity: this group includes all emissions from UO3 caused by every input but electricity.

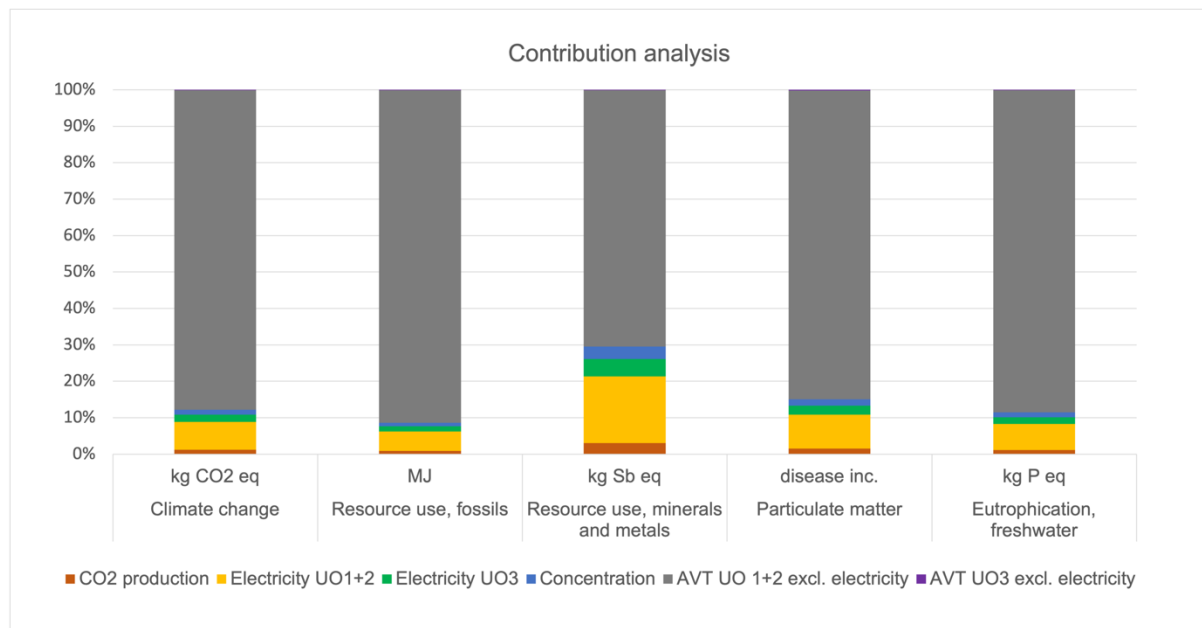


Figure 4: Contribution analysis of the WaterProof formic acid production (base scenario)

The hotspot analysis revealed that in all investigated impact categories, UO1+2 excl. Electricity is the most contributing process component, with the majority of loads/impacts originating from the use of potassium hydroxide, which is an essential chemical for UO1 and subsequent UO2. The contribution of UO1+2 (excl. energy, mainly KOH) in the climate change impact category is 89%. With 92% the maximum contribution of UO1+2 is in the impact category resource use fossil. The dominant contribution is primarily attributable to the fossil-based background processes of KOH, but also to the fact that renewable electricity is assumed in this baseline scenario, which has a very low impact on the overall process with a GWP of 0.016 kg CO₂ eq./kWh. All process components related to energy together only contribute between 7.9% and 27% in the five impact categories. The latter is the contribution to the impact category resource use minerals and metals. The higher proportion can be explained by the background data sets for wind energy, as copper, steel and cast iron are used here. All absolute results for the contribution analysis can be found in Table 6.

Table 6: Absolute impacts of 1 kg formic acid production

Impact category	Unit	Sum	CO ₂ production	Electricity UO1+2	Electricity UO3	Concentration	UO1+2 excl. electricity	UO3 excl. electricity
Climate change	kg CO ₂ eq/kg	0.28	0.00	0.02	0.01	0.00	0.25	0.00
Resource use, fossils	MJ/kg	4.55	0.04	0.24	0.06	0.04	4.15	0.01
Resource use, minerals and metals	kg Sb eq/kg	4.22E-06	1.27E-07	7.72E-07	2.02E-07	1.42E-07	2.97E-06	5.49E-09
Particulate matter	Disease inc./kg	1.82E-08	2.79E-10	1.70E-09	4.44E-10	3.13E-10	1.54E-08	3.90E-11
Eutrophication, freshwater	kg P eq./kg	1.27E-04	1.49E-06	9.05E-06	2.37E-06	1.67E-06	1.1267E-04	1.62E-07

In order to classify the results of the hotspot analysis for the 5 impact categories evaluated, three scenarios were analysed and compared with the baseline scenario. The three other scenarios are described in the next section and then compared for each impact category.

5.3 Benchmark and scenario analysis

The overall impact assessment results shown in the hotspot analysis can be compared to a benchmark and other scenarios, which will be described in the following. All benchmarks and scenarios are evaluated based on the same functional unit described in 3.2.3.

Benchmark fossil-based formic acid (renewable electricity)

An ecoinvent dataset for the European production of fossil-based formic acid was used which represents the production of 1 kg of formic acid by hydrolysis of methyl formate, which is obtained by carbonylation of methanol (Formic acid {RER}| formic acid production, methyl formate route | Cut-off, U). For a fair comparison, the datasets related to electricity for the production of the input data (methanol and carbon monoxide) as well as for the formic acid production has been exchanged to the same dataset which was used for electricity in the WaterProof dataset (Electricity, high voltage {NL}| electricity production, wind, 1-3MW turbine, offshore | Cut-off, U). In addition, a formic acid concentration of 30wt% was assumed.

WaterProof formic acid (grid mix electricity)

This scenario reflects the current European electricity supply from the grid mix. It corresponds to the same model as the baseline scenario, except for the dataset for

electricity, and the following ecoinvent dataset was used for the modelling: Electricity, medium voltage {RER}| market group for electricity, medium voltage | Cut-off, U. The contribution analysis of this scenario can be found in Annex B.

Benchmark fossil-based formic acid (grid mix electricity)

This scenario represents the fossil-based formic acid production with the current European electricity supply from the grid mix. The following dataset has been used: Formic acid {RER}| formic acid production, methyl formate route | Cut-off, U. For a fair comparison, a formic acid concentration of 30wt% was assumed.

5.3.1 Characterised results

The characterised relevant EF 3.1 investigated potential impacts are reported in Table 7 and

Table 8. The WaterProof baseline scenario was compared with the fossil-based benchmark. Renewable electricity was used as the energy source in both models. To give an indication of how the WaterProof process performs in the current European electricity mix, both models were also modelled with a European electricity mix dataset. It was clearly shown that the highly electricity-based WaterProof process is only more favourable if renewable energy is used for the process. While differences between 6% and 68% could be achieved in all five impact categories with renewable energy, the use of the grid mix shows disadvantages in four out of five impact categories.

Table 7: Characterised results for 30wt% WaterProof FA and fossil-based FA with renewable electricity

Impact category	Unit	WaterProof FA (renewable electricity)	Fossil-based FA (renewable electricity)	Difference
Climate change	kgCO ₂ eq./kg	0.28	0.65	-57.0%
Resource use, fossils	MJ/kg	4.55	14.23	-68.0%
Resource use, minerals and metals	kg Sb eq./kg	4.22E-06	4.50E-06	-6.3%
Particulate matter	Disease inc./kg	1.82E-08	2.24E-08	-18.7%
Eutrophication, freshwater	kg P eq./kg	0.00013	0.00021	-39.0%

Table 8: Characterised results for 30wt% WaterProof FA and fossil-based FA with European grid mix electricity

Impact category	Unit	WaterProof FA (grid electricity)	Fossil-based FA (grid electricity)	Difference
Climate change	kgCO ₂ eq./kg	0.99	0.82	19.5%
Resource use, fossils	MJ/kg	21.03	18.22	15.4%
Resource use, minerals and metals	kg Sb eq./kg	4.43E-06	4.55E-06	-2.7%
Particulate matter	Disease inc./kg	2.79E-08	2.47E-08	12.9%
Eutrophication, freshwater	kg P eq./kg	0.00078	0.00036	112.7%

5.3.2 Climate change

Comparing the environmental impact on climate change of WaterProof's formic acid with that of fossil-based formic acid reveals significant differences. Figure 5 shows the different scenarios in comparison. The WaterProof baseline scenario formic acid (with renewable electricity) has a 57% lower impact on climate change compared to the fossil-based

benchmark (also with renewable electricity). However, when comparing the other two scenarios, which use a European energy grid mix (351 g CO₂ eq./kWh) instead of renewable energy (15 g CO₂ eq./kWh), it is noticeable that the WaterProof process has a higher environmental impact than the fossil-based production of formic acid. This is due to the fact that the electrochemical production of formic acid in the WaterProof process requires almost exclusively electricity as energy source, whereas fossil-based FA also requires a lot thermal energy (heat from natural gas). In addition, the WaterProof process is still in development (TRL 6 shall be reached at the end of the project), whereas the fossil-based formic acid process is a conventional process which is used as a high scale and has been optimised since decades. As a result, the impact in the WaterProof process using current electricity mix is much stronger than in the benchmark process. Figure 5 clearly shows how important it is for the WaterProof process to run on renewable energy, as otherwise it will have a higher environmental impact in terms of climate change than the benchmark.

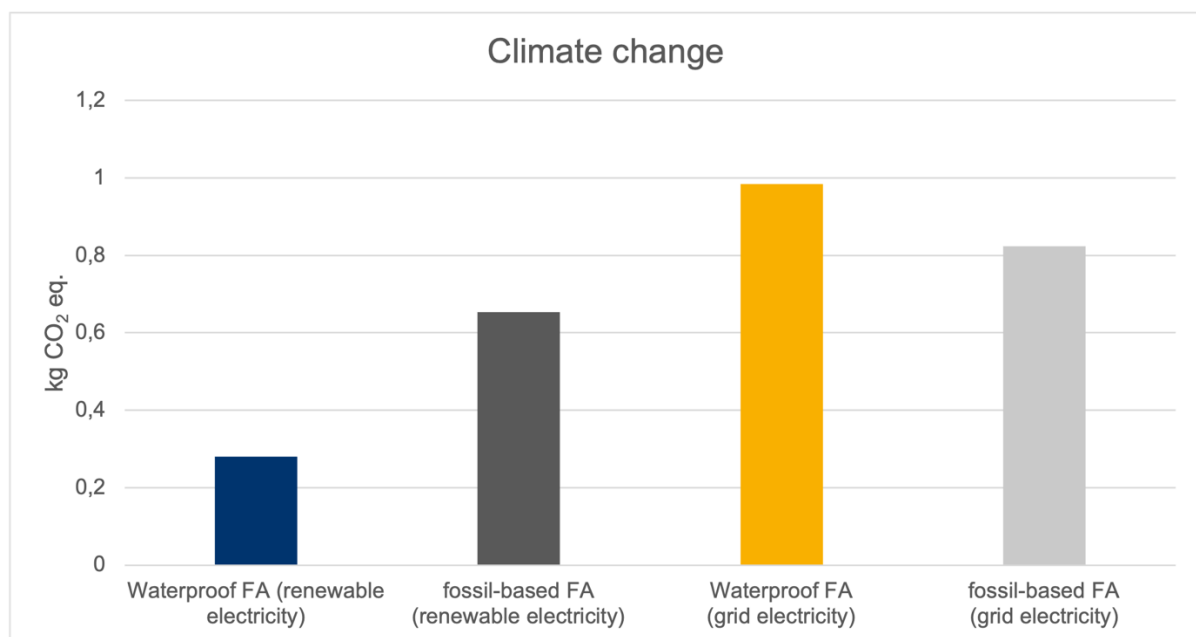


Figure 5: Environmental impact category climate change – scenario and benchmark comparison

5.3.3 Resource use, fossils

Similar results can be derived for the utilisation of fossil resources (**Error! Reference source not found.**). The difference between WaterProof FA (renewable electricity) and WaterProof FA (grid electricity) is due to the change in energy intensity. The production of potassium hydroxide contributes in both scenarios approx. 4 MJ to the systems, the rest

can be attributed to the electricity usage during the process. As renewable energy is used in the baseline scenario, the energy inputs for the process contribute very little to fossil resource utilisation. Conversely, using the grid electricity mix leads to higher fossil resource utilisation, because the grid electricity mix also contains electricity generating processes based on the use of fossil resources. However, the main contributor for the benchmark is the fossil-based feedstock carbon monoxide so that a switch to renewable electricity is not as strong as in the Waterproof process.

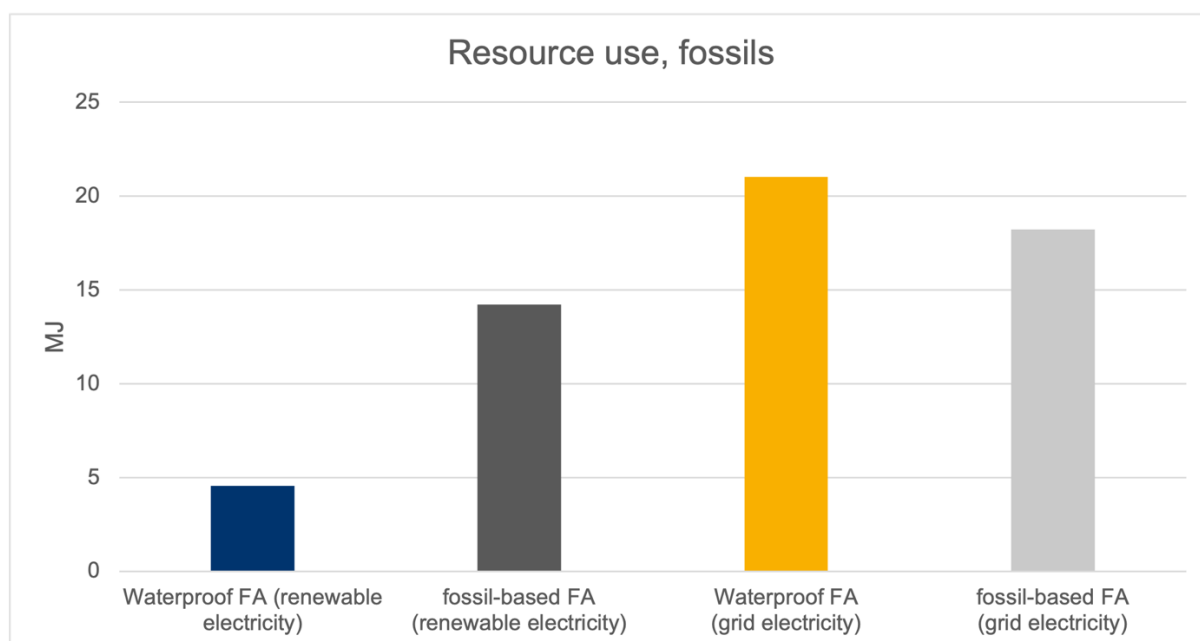


Figure 6: Environmental impact category resource use, fossils – scenario and benchmark comparison

5.3.4 Resource use, minerals and metals

The comparison of the resource use of minerals and metals is depicted in Figure 7. The baseline Waterproof process has the lowest contribution in this category. The impacts in this category arise mainly due to background datasets in potassium hydroxide production (mainly copper cathode). For the fossil-based FA, the impacts can also be attributed to the background datasets of the feedstock carbon monoxide and chemical factory organics (also copper cathode). The deterioration of the values in the grid mix scenario can be explained by the increased use of copper cathodes within the electricity dataset in comparison to the dataset used for renewable electricity.

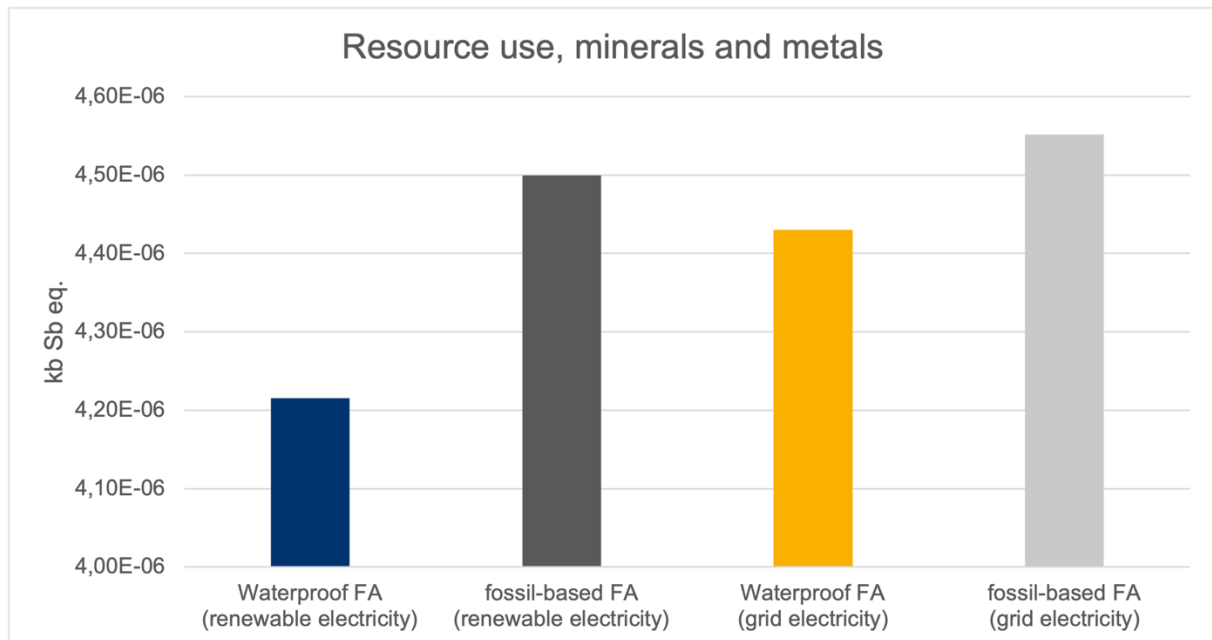


Figure 7: Environmental impact category resource use, minerals and metals – scenario and benchmark comparison

5.3.5 Particulate matter

The emissions that have an impact in the environmental category particulate matter all originate from background datasets. In the baseline scenario, emissions from potassium chloride production cause particulate matter in the background. The emissions from fossil-based FA are almost entirely attributable to background data from heat generation. In the WaterProof scenario with European grid electricity, the impact from the fossil-based electricity in combination with the impact of potassium chloride production also contributes to the higher result. The results are shown in Figure 8.

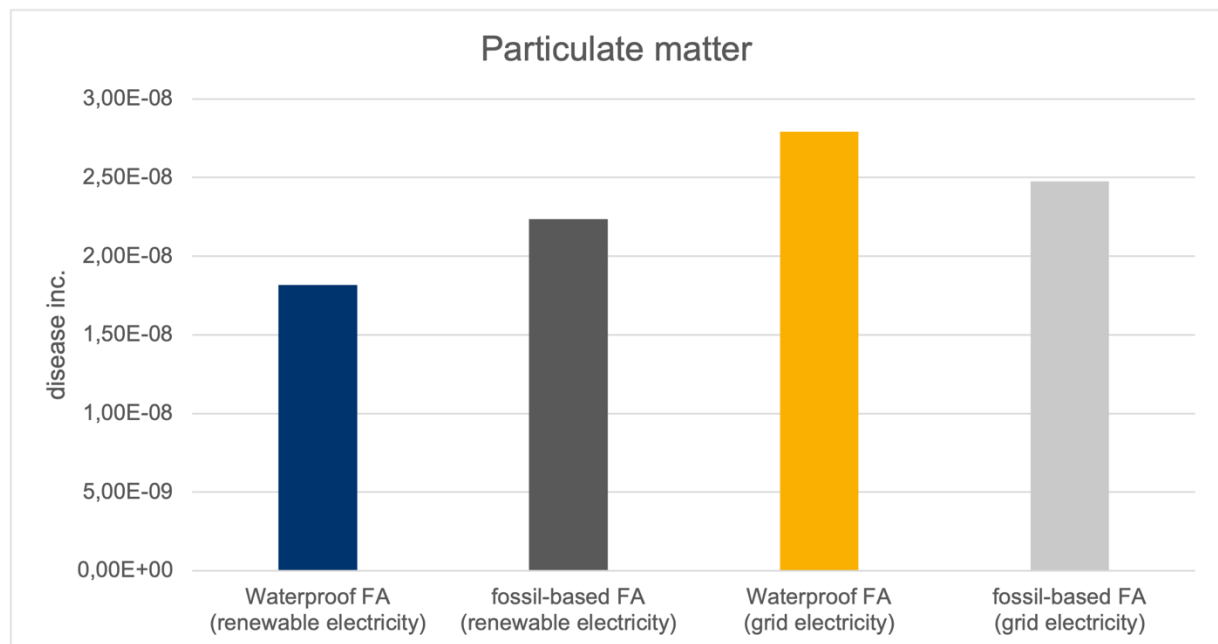


Figure 8: Environmental impact category particulate matter – scenario and benchmark comparison

5.3.6 Eutrophication, freshwater

The emissions in the impact category eutrophication freshwater in the WaterProof process are almost entirely attributable to energy background datasets in potassium hydroxide production, which go back to the spoil from hard coal and lignite mining, which subsequently leads to groundwater contamination, including the leaching of compounds such as sulphur and other chemicals by precipitation. The same applies to fossil-based FA for which the electricity background datasets of carbon monoxide production (spoil from hard coal mining and spoil from lignite mining) are the cause of the emissions. The large difference between the WaterProof baseline scenario and the WaterProof grid electricity scenario is therefore understandable as the grid mix uses significantly more electricity from non-renewable sources, which leads to more spoil from lignite and hard coal and the associated higher emissions. The results are shown in Figure 9.

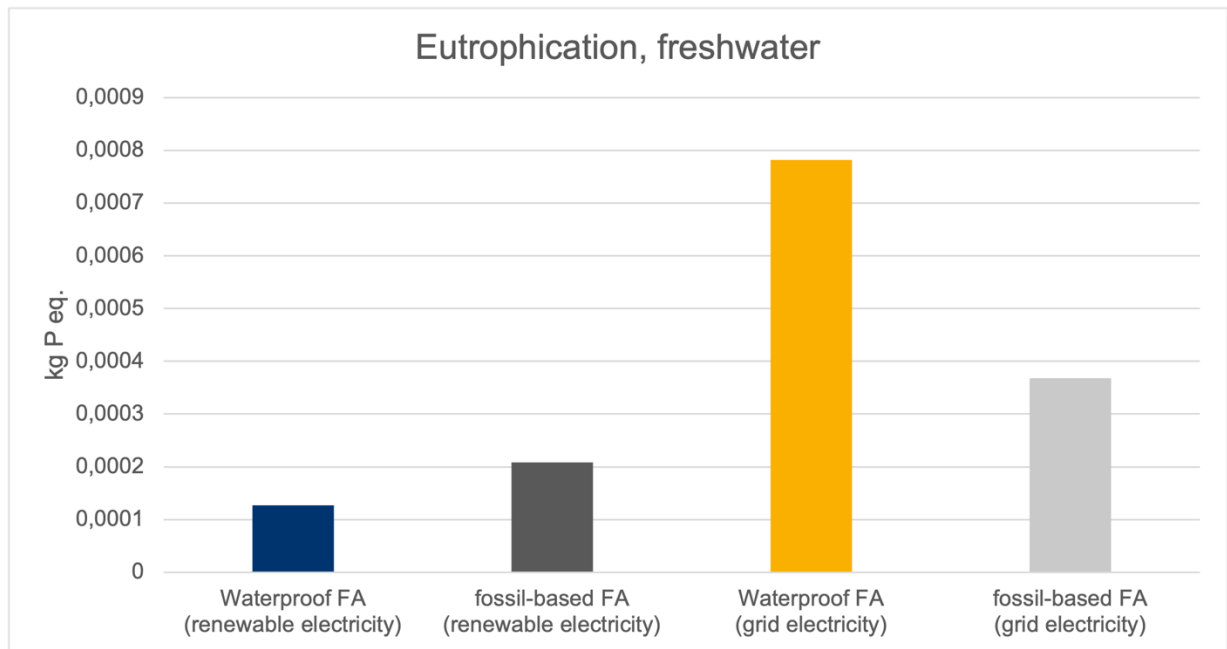


Figure 9: Environmental impact category eutrophication, freshwater – scenario and benchmark comparison

6 Conclusion

Based on the analyses in previous chapters, the following conclusions can be drawn:

- The results of this LCA give an early understanding of the environmental performance of the WaterProof process at its current stage of development. The identification of hotspots at this stage is of great importance, since it can lead to the identification of approaches to mitigate the impacts and can help take decisions for further selection and the development of CO₂-based formic acid with improved environmental profile. The results are only preliminary and the comparison with the benchmark only serves as an initial assessment. According to ISO 14040/14044, a correct comparison must be reviewed critically
- The LCA conducted for this study is subject to several limitations and sources of uncertainties. Firstly, as the assessed processes are still in the early stages of development, the availability of life cycle inventory data and the accuracy of environmental evaluations are uncertain. While these uncertainties are expected to decrease as the project progresses, it's crucial to acknowledge the evolving nature of the data. Additionally, comparisons to the benchmark, particularly in contrast to the commercially established and optimized petrochemical-based formic acid production, must be approached with caution under this limitation. Secondly, uncertainties in foreground processes arise from the data derived from the maximum capacity of UO3. Consequently, the validity of the study's results is confined within the context of this assumption, emphasizing the importance of recognizing and accounting for such limitations. Lastly, while efforts were made to utilize the best available background datasets from the Ecoinvent LCA database, uncertainties persist. Although the overall selection of datasets was rated as good, complete exclusion of uncertainties is unattainable. These uncertainties in background data necessitate a cautious interpretation of the study's findings. Overall, acknowledging these limitations and sources of uncertainties is essential for ensuring the robustness and reliability of the LCA outcomes.
- LCA is a methodology based on multiple choices and for each input many scenarios are possible (e.g. different feedstocks, different energy supply options, different methodological options...). For this initial screening one baseline scenario was defined for the WaterProof process as a starting point of the evaluations, which can help identify meaningful scenarios worth of a closer look. For instance, the

contribution of electricity to the environmental impacts was proven to be dominating.

- The climate change, resource use of fossil fuels and resource use of minerals and metals were found to be predominately the most relevant categories contributing to the environmental impact of the WaterProof process. The first two indicators (climate change and resource use of fossil fuels) are also the most relevant indicators in the current political agenda driving the transition from fossil to renewable carbon. In addition, and to a lesser extent, particulate matter and eutrophication of freshwater were also identified as relevant categories within the product systems under study.
- Hotspot analyses showed that most of the impacts arise from the upstream of potassium hydroxide, being the energy and steam supply (for potassium chloride) as the dominating environmental hotspot. If potassium hydroxide is also produced using renewable energy, the impact on climate change would be lower, but KOH would still be the hotspot for the WaterProof process.
- A benchmarking of the environmental performance of WaterProof's formic acid against potential fossil-based formic acid is also provided, and both products are compared with renewable electricity and grid mix electricity. The comparison showed that the formic acid produced in the WaterProof process has a lower environmental impact in all five evaluated impact categories as long as the process is carried out using renewable energy. For example, WaterProof's formic acid production process releases less GHG emissions (57%) than fossil-based formic acid production (0.28 vs. 0.65 kg CO₂ eq./kg). When applying today's European electricity mix the scenario analysis depicted that the fossil-based process shows lower emissions in four out of five impact categories (e.g., climate change: WaterProof's formic acid 0.99 kg CO₂ eq./kg and fossil-based formic acid 0.82 kg CO₂ eq./kg). Note that this is a preliminary insight of WaterProof environmental preferability and that a proper comparison which is made publicly available shall undergo a critical review to be considered as conform to ISO 14040/14044.
- In order to further develop or improve the environmental performance of WaterProof's formic acid it is crucial that the use of KOH is as efficient as possible, as this is the hotspot of all environmental impacts. Since KOH is produced in UO3,

it can be used again in UO1. The reuse of the KOH produced in UO3 and the associated lower environmental impacts were not yet considered in this LCA, as the data for UO3 had not yet been measured. Actual data will be available in the further course of the project so that this utilisation will also be considered in the final report on LCA towards the end of the project and included in D4.8.

- It must also be emphasised that the LCA focuses only on the environmental aspect of sustainability. A full sustainability assessment should also consider technical, economic and social aspects. These aspects are also being tracked and evaluated in task 4.2, 4.3 and 4.4 of WP4 and reported as D4.2 and D4.3.

7 List of abbreviations

Abbreviation	Description
ADES	Acetic deep eutectic solvent
AVT	Avantium
C	Carbon (atomic)
CH	Switzerland
CTUe	Comparative Toxic Units (ecosystems)
CTUh	Comparative Toxic Units (humans)
EC	European Commission
EF	Environmental Footprint
e.g.	Example given
Eq.	Equivalent
FA	Formic acid
FU	Functional unit
GHG	Greenhouse gases
HCOOH	Formic acid
H ₂ O	Water
i.e.	That is
ISO	International Organisation for Standardisation
KOH	Potassium hydroxide
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
N	Nitrogen (atomic)
NL	The Netherlands
NMVOC	Non-Methane Volatile Organic Compounds
NO _x	Nitrogen oxides
O	Oxygen (atomic)
P	Phosphorous (atomic)

Pt	Production per m ² and year (land use)
RER	Europe
S-LCA	Social Life Cycle Assessment
TEE	Techno economic evaluation
U	Unit process (Ecoinvent datasets)
UO	Unit Operation
U-235	Uranium isotope 235
WP	Work Package
WWTP	Waste Water Treatment Plant

8 References

Ecoinvent (2024): Ecoinvent, Ecoquery Version 3.9. Available online at ecoinvent.org.

EF (2022): Environmental Footprint version 3.1. Impact assessment method of the European Environmental Footprint initiative.

ISO (2006a): Environmental management - Life cycle assessment - Principles and framework (ISO 14040:2006).

ISO (2006b): Environmental management - Life cycle assessment - Requirements and guidelines (ISO 14044:2006); German and English version EN ISO 14044:2006.

9 Annex

Annex A – background datasets

Table 9: Used datasets

Background datasets	Datasets	Source	Year
Renewable electricity	Electricity, high voltage {NL} electricity production, wind, 1-3MW turbine, offshore Cut-off, U	Ecoinvent 3.9	2015
European grid electricity	Electricity, medium voltage {RER} market group for electricity, medium voltage Cut-off, U	Ecoinvent 3.9	2015
water	Water, deionised {Europe without Switzerland} water production, deionised Cut-off, U	Ecoinvent 3.9	2017
KOH	Potassium hydroxide {RER} potassium hydroxide production Cut-off, U	Ecoinvent 3.9	2018

Annex B – contribution analysis

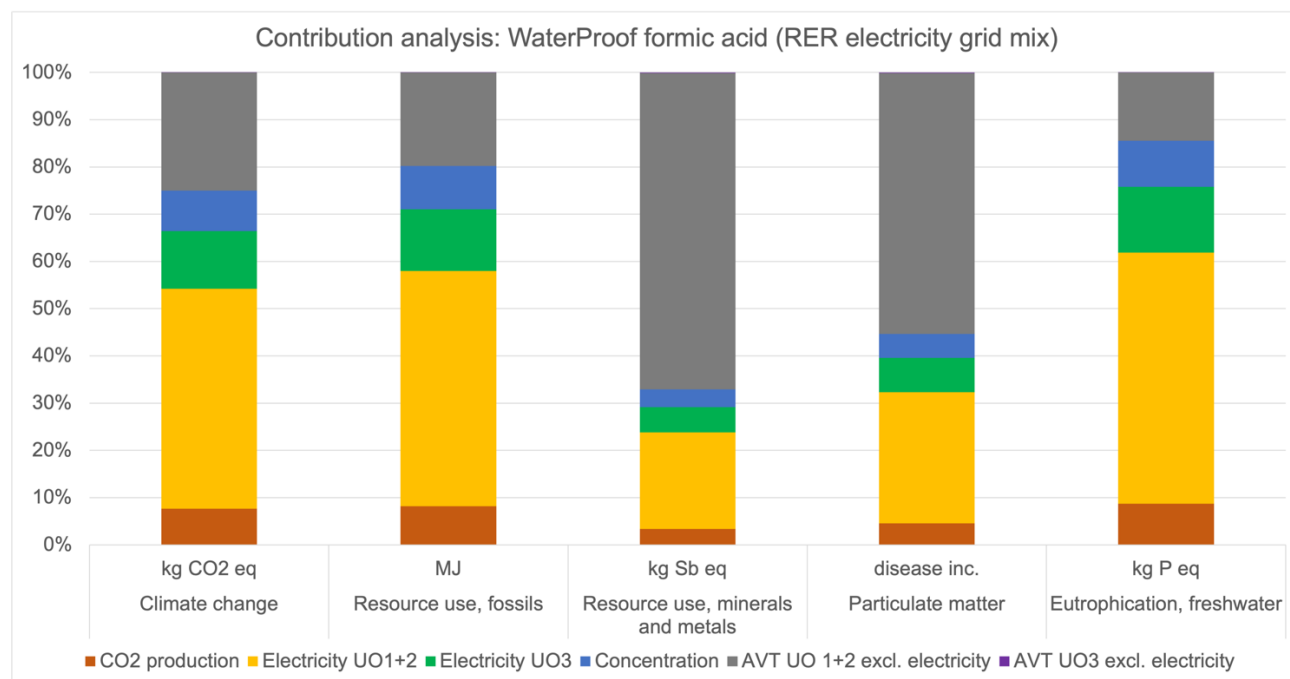


Figure 10: Contribution analysis of the WaterProof formic acid production using European electricity grid mix