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ZEROF

D6.1 Report on safe- and sustainable-by-design methodological framework

Deliverable D6.1

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Executive Summary

The ZeroF project intends to apply the "safe and sustainable by design" (SSbD) framework developed by the European Commission to support the development of the per- and polyfluoroalkyl substances (PFAS) alternatives for the packaging and textile coating applications and ensure their safety and sustainability. This deliverable describes how the SSbD framework will be applied within ZeroF project, including the methodological background of the different steps and how they will be applied to each ZeroF sectoral application.

While applying relevant design principles (e.g., waste recovery, energy efficiency), the safety and sustainability performances of the new materials and the design alternatives will be evaluated following the different steps defined by the EC framework. Safety will be evaluated based on three safety steps (hazard assessment, safety risks along production and processing steps, and safety risks for the final application) using publicly available data, but also filling data gaps thanks to experimental hazard testing and the use of computational models. For environmental sustainability (step 4), life cycle assessment (LCA) methodology will be applied, investigating potential missing characterization factors for (eco-)toxic substances and the definition of criteria aligned with the planetary boundaries concept. The economic sustainability assessment in step 5 will be based on life cycle costing (LCC) methodology, where the same settings than for the LCA will be applied for a harmonized assessment. These assessments will be performed in an iterative manner along the project to support design choices, where several aggregation approaches will be tested to rank the possible options. Besides this, the social acceptance of the ZeroF materials will be evaluated based on surveys and interviews. However, the related results will not be used to steer design choices (only one final evaluation).

To apply the SSbD methodology to the materials developed for packaging and textile coating, several modelling choices were made. First, the life cycle approach is applied but potential processes or flows which do not affect the results could be excluded (e.g., transport). The life cycle steps can be divided into coating material synthesis, coating and finishing processes, and use and disposal of the final product. For the LCA and LCC evaluation, the reference flow of 1 m^2 of coated product (packaging or textile) will be used while the functional unit additionally includes the targeted performances (water and oil repellence). The reference scenario considered will be the common PFAS compound used in each of the application, but more ambitious targets will be defined along the project to move towards an "absolute" assessment. The investigated design alternatives concern the use of different raw materials, additives or operating conditions for the material synthesis but also the type of coating process. To efficiently collect data for the SSbD evaluation, a common Excel file was prepared to collect the necessary data for the safety, environmental and economic sustainability assessment, keeping track of data quality.

The ZeroF consortium will follow the future developments on European level (revision of the EC framework expected in 2025) and synchronise the ZeroF SSbD framework as deemed necessary.

Keywords

SSbD, design principles, safety, sustainability, coating materials

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Abbreviations and acronyms

Acronym	Description
4:2 FTOH	4:2 fluorotelomer alcohol
CeFAE	Cellulose fatty acid ester
CF	Characterization factor (used in LCIA to convert flows into impacts)
CSS	Chemicals Strategy for Sustainability
DWR	Durable water repellent
EC	European Commission
FDA	Food and Drug Administration
ISO	International organisation for standardisation
JRC	Joint Research Centre
LCA	Life cycle assessment
LCC	Life cycle costing
LCI	Life cycle inventory
LCIA	Life cycle impact assessment
MCI	Material circularity indicator
PFAA	Perfluoroalkyl acid
PFAS	Per- and polyfluoroalkyl substance
PFBS	Perfluorobutane sulfonic acid
PFHxA	Perfluorohexanoic acid
PFOA	Perfluorooctanoic acid
R&I	Research and innovation
SSbD	Safe and Sustainable by Design
SVHC	Substance of very high concern
TAM	Technology acceptance model
TRL	Technology readiness level
VOC	Volatile organic compound
VRE	Value-based resource efficiency
WP	Work Package

1 Introduction

Within the European Green Deal, the European Commission (EC) adopted in October 2020 the Chemicals Strategy for Sustainability (CSS) to mainly support the "zero pollution" ambition (EC, 2020). Indeed, the CSS aims at phasing out the most harmful substances and thus promoting the production and use of safer and more sustainable alternatives. While increasing safety is the first concern of the CSS, other sustainability aspects are also considered to contribute to other pillars of the European Green Deal, such as the climate neutrality or circular economy. The objective is also to adopt a life cycle approach to understand the impact along the different stages of the materials, from production to use and disposal, and thus avoid regrettable substitution thanks to a comprehensive approach.

To reach the CSS ambitions, the Joint Research Centre (JRC) developed a framework to develop "safe and sustainable by design" (SSbD) chemicals and materials and thus support research and innovation (R&I) activities for the development of alternatives. The JRC framework was published in 2022 (Caldeira et al., 2022a), which was officially released by the EC on December 8, 2022 (EC, 2022). The EC SSbD framework defines the general approach, provides guidance for the definition of safety and sustainability criteria, and describes the related evaluation procedures. This framework is currently under the 1st testing period. The EC will collect feedback from stakeholders (during Q2 of 2023 and of 2024) to provide a revised version in 2025.

The ZeroF project intends to apply the EC SSbD framework to support the development of the per- and polyfluoroalkyl substances (PFAS) alternatives for the packaging and textile coating applications and ensure their safety and sustainability. This deliverable describes how the SSbD framework will be applied within ZeroF project. An overview of the methodological background is provided in section 2, followed by a detailed description of the settings of the SSbD framework (i.e., definition of system boundaries, scenarios and data requirements) for each ZeroF sectoral application in section 3.

2 SSbD methodology

SSbD aims at guiding the design of new materials and verify their compliance with safety and sustainability criteria. The framework has thus two components:

- The **(re)design phase** where design guiding principles can support design choices based on practical actions and technical indicators to monitor the implementation of these actions (e.g., material efficiency guiding principle can be achieved by improving the recovery of unreacted chemicals, which can be then measured by the net mass of materials consumed and the recovery rate).
- The **safety and sustainability assessment** phase where these dimensions and related indicators are evaluated to check their alignment with criteria and thus identify if new design alternatives need to be investigated (if trade-offs were observed) or if further development can continue.

This stepwise approach is intended to be applied along the innovation processes, from low technology readiness levels (TRL) to the final market deployment, to be able to identify as soon as possible safety or sustainability issues, and thus facilitate the implementation of corrective actions. The SSbD framework is thus a continuous process with several iterations along the various innovation steps.

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Besides this, the EC adopted a hierarchical approach between the dimensions, with safety aspects considered first (due to the main objective of the CSS), followed by environmental, social and economic aspects. The methods to support socio-economic sustainability are less mature, which explains why the EC considers their evaluation as an optional step for now.

The following sub-sections details the SSbD methodologies used in ZeroF, following the EC framework, starting with the guiding design principles (section 2.1). Then, the five steps for the safety and sustainability assessment are described:

- **Step 1** – Hazard assessment of the chemical/material
- **Step 2** – Human health and safety aspects in the chemical/material production and processing phase
- **Step 3** – Human health and environmental aspects in the final application phase
- **Step 4** – Environmental sustainability assessment (section 2.3)
- **Step 5** – Social and economic sustainability assessment

For convenience, the steps 1, 2 and 3 are grouped into one single sub-section dealing with safety evaluation (section 2.2), while the economic and social sustainability assessment are divided into two parts (sections 2.4 and 2.5).

The last sub-section (2.6) provides a short introduction to the integration of the evaluation results of the SSbD methodology produced during the 5 steps of the framework and how the project consortium aims at integrating the results of the case studies for extracting consolidated results.

2.1 Guiding design principles

The SSbD framework intends to support the design of new chemicals or materials, at the molecular level (influencing the intrinsic properties of the new substances), process level (investigating the production operating conditions) or at product level (in which the new chemical/material is integrated). To do so, the EC promotes guiding principles which should contribute to better safety and sustainability performances (this should always be verified via the subsequent steps of safety and sustainability assessment).

Based on previous scientific initiatives, such as the green chemistry, green engineering, sustainable chemistry or safe by design principles, a set of eight design principles were defined (Table 1). Depending on the feasibility, these principles can be followed by the material developers. It is important to highlight that a material can be promoted as a "SSbD material" only if it complies with safety and sustainability criteria, evaluated with the following steps, while the eight design principles only have a guidance role to increase the chance to be compliant with the safety and sustainability criteria. This support role is emphasized by the fact that the EC makes it optional to report the adherence to SSbD principles.

For each SSbD principle, a short definition and examples of actions to implement it and of indicators to monitor it are provided in Table 1. The indicators are related to technical design aspects, which the material developers can easily relate to. Some of them refer to circularity aspects, such as the recycled content and the share of renewable energy for SSbD4, the ability to recycle the material for SSbD7 or the value-based resource efficiency (VRE) and the material circularity indicator (MCI) for SSbD8. These circularity indicators will also be calculated in ZeroF project for the investigated design alternatives.

Table 1: SSbD Design guiding principles from the EC (non-exhaustive list of examples of actions and indicators, Caldeira et al. 2022a)

SSbD principle	**Definition**	**Examples of actions**	**Examples of indicators**
SSbD1 Material efficiency	Reducing the use of raw materials and the generation of waste	- Maximise reaction yield - Recover unreacted chemicals - Optimise solvent for purpose	- Net mass of materials consumed (kg/kg) - Reaction yield - Total amount of waste (kg/kg)
SSbD2 Minimise the use of hazardous chemicals/materials	Preserve functionality while reducing or avoid using hazardous materials	- Eliminate hazardous materials - Analysis of using hazardous materials in close loops	- Classification of raw materials as SVHC - Biodegradability of manufactured chemical/material (yes/no)
SSbD3 Design for energy efficiency	Minimise the overall energy used to produce/process a chemical/material	- Maximise energy re-use (e.g., heat networks integration) - Fewer production steps	- Energy consumption (kWh/kg or MJ/kg) - Boiling temperature (°C) - Energy efficiency (%)
SSbD4 Use renewable sources	Closing the loops or using renewable or secondary material and energy sources	- Select renewable or secondary materials that do not create land competition and/or processes - Use renewable energy sources	- Share of renewable feedstock (%) - Share of renewable energy (%) - Recycled content (%)
SSbD5 Prevent and avoid hazardous emissions	Apply technologies to minimise or avoid hazardous emissions	- Select materials and/or processes that minimise the generation of - Hazardous waste - Emissions (e.g., VOCs, metals)	- Critical air mass (%) - Biological oxygen demand (g/kg) - Wastewater to treatment (m^3/kg) - Amount of hazardous waste (kg/kg)
SSbD6 Reduce exposure to hazardous substances	Eliminate exposure to chemical hazards (combine SSbD2 and SSbD5)	- Avoid as much as possible SVHC - Consider value chain regulations - Eliminate hazardous substances	- Classification of raw materials as SVHC - Biodegradability of manufactured chemical/material (yes/no)
SSbD7 Design for end-of-life	Design chemicals/ materials so that waste products do not pose any risk and do not hinder reuse, sorting and recycling/upcycling	- Avoid chemicals that hamper the recycling processes - Select materials that are more durable, easy to separate or truly biodegradable	- Recyclable? (yes/no) - Durability (years) - Disassembly/reparability design (yes/no)
SSbD8 Consider the whole life cycle	Apply the other design principles through the entire life cycle	- Using reusable packaging along the supply chain - Energy-efficient logistics - Responsible sourcing principles	- Value-based resource efficiency indicator - Material circularity indicator (MCI) - Durability (years)

2.2 Safety assessment

Safety assessment following the European Commission approach is divided into 3 steps as indicated below.

2.2.1 Step 1 Hazard Assessment of the chemical/material

This step deals with the intrinsic hazard of a chemical, or hazard level, and is aligned with the EU Zero Pollution Action Plan and the Chemicals Strategy for Sustainability, both seeking to better protect citizens and the environment from hazardous chemicals and pollution. The approach to implement this step is to follow the Classification, Labelling and Packaging (CLP) Regulation ((EC) No 1272/2008), which harmonises criteria to classify chemicals that are hazardous according to their intrinsic physico-chemical, toxicological and ecotoxicological properties. To collect such information, one may use the European Chemicals Agency database (https://www.echa.europa.eu/information-on-chemicals), as well as similar databases such as PubChem (https://pubchem.ncbi.nlm.nih.gov/), SubsPortPlus (https://www.subsportplus.eu/) and many more portals/tools (QSAR toolbox, AMBIT, Chemsec Sinlist) or national/international entries (Dutch SVHC portal, JRC EASIS portal, Danish Endocrine disruptor list). The European Commission recommends to group chemicals in three categories, e.g., most harmful substances, substances of concern and other hazard classes (Table 2). Following this approach, hazard information on all reagents should be available, otherwise it is not possible to conclude that reagents are safe. For this step 1, the SSbD follows the scheme shown in Figure 1. This step allows for the identification of data gaps and the implementation of testing strategies to cover for those. Once all data is available, an assessment can be put in place and conclusions on whether to go to the next step or look for chemical replacement may be taken. In cases where data scarcity may hamper the hazard assessment of chemicals/materials, the ZeroF consortium aims to complement the assessment with experimental activities by performing within WP6 *in vitro* hazard testing and computational modelling for producing data for gap filling. WP5 aims to support the assessment by providing automatic gap filling tools based on existing and project generated data.

Table 2: Group of substances to consider for regulatory compliance (Caldeira et al.2022b)

Group of substances	Human health hazards	Environmental hazards	Physical hazards
Most harmful substances according to CSS (REF), including substances of very high concern (SVHC) according to REACH Art. 57 (REF)	Carcinogenicity, Germ cell mutagenicity, Reproductive / developmental toxicity: Cat. 1A & 1B Endocrine disruption, Respiratory sensitisation, Specific target organ toxicity – repeated exposure: Cat.1	Persistent, bioaccumulative and toxic/very persistent and very bioaccumulative (PBT/vPvB) Persistent, mobile and toxic/very persistent and mobile (PMT/vPvM) Endocrine disruption Cat. 1	
Hazardous substances with chronic effect, part of the substances of concern described in CSS (REF)	Skin sensitisation Cat. 1 Carcinogenicity, Germ cell mutagenicity, Reproductive / developmental toxicity, Specific target organ toxicity – repeated exposure, endocrine	Hazardous for the ozone layer Chronic environmental toxicity (chronic aquatic toxicity) Endocrine disruption Cat. 2	

	disruption: Cat. 2 Specific target organ toxicity – single exposure: Cat. 1 & 2		
Other hazard classes	Acute toxicity Skin corrosion Skin irritation Serious eye damage / eye irritation Aspiration hazard (Cat. 1) Specific target organ toxicity – single exposure Cat. 3	Acute environmental toxicity (acute aquatic toxicity)	Explosives Flammable gases, liquids and solids Aerosols Oxidising gases, liquids and solids Gases under pressure Self-reactive Pyrophoric liquids and solids Self-heating In contact with water emits flammable gas Organic peroxides Corrosivity Desensitised explosives

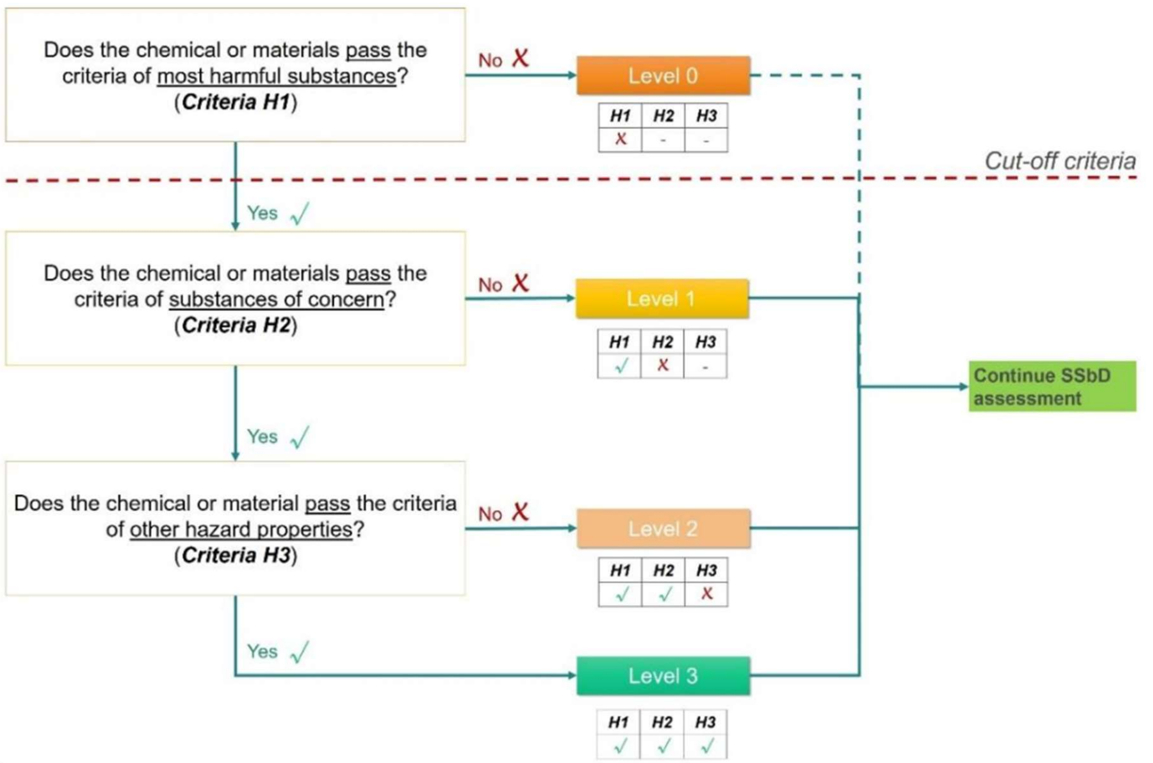

Figure 1: Strategy to Implement Step 1 of the SSbD Framework

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2.2.2 Step 2 Human health and safety aspects in the chemical/material production and processing phase

This step deals with the identification of risk to workers (Occupational safety). There is currently an inventory of tools used in the EU which may assist with this step (European Regional Chapter of the International Society on Exposure Science (ISES Europe)). To perform this step, exposure to the chemicals must be collected. If data is not available, information needs to be collected following tools such as the ECETOC TRA[1] or the Use Maps, which have been developed by sector associations to provide information in a harmonised way on the manufacturing processes and operational conditions for the production of their products using a series of descriptors[2]. Information about the processes and operational conditions can also be gathered in the supply chain. Based on the collected information, including conditions use, the corresponding exposure estimates are calculated and compared with the predicted no-effect concentrations for the environment (PNECs) and the derived no-effect levels for human health (DNELs).

A series of questions may be asked to collect information:

-How is the substance produced?

- batch process;
- continuous process.

-Where is the substance produced?

- enclosed processes or plants;
- indoor controlled environment;
- indoor open sources;
- outdoor; etc.

-What are the operational conditions?

- characteristics of the substance (physical state/dustiness/vapour pressure) and its concentration in a mixture or material under the operational conditions;
- duration and frequency of the activity;
- duration and frequency of exposure;
- temperature of the process; etc.

-What are the risk management measures (RMM) in place?

- General ventilation;
- Local exhaust ventilation;
- General occupational safety and health (OSH) management systems (e.g., housekeeping, training…);
- personal protective equipment (PPE).

-How is the substance used?

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1 https://www.ecetoc.org/tools/tra-main/https://www.ecetoc.org/tools/tra-main/
2 https://echa.europa.eu/csr-es-roadmap/use-maps/concept

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- high energy processing (e.g., spraying, grinding, hot processes) or low energy processing (e.g., assembly of article components, dipping of articles into vat);
- remote or intimate contact during normal operation; etc.

2.2.3 Step 3 Human health and environmental aspects in the final application

This step looks into potential risks to consumers and the environment due to the product use. To perform this step, it is important to identify the corresponding regulation, such as in the case of ZeroF one may refer to Regulation 10/2011 (EC, 2011) on plastic materials and articles intended to come into contact with food. This regulation guides us to health risks which exist due to the intake of a substance with a certain hazard potential. Intakes refer to exposure which, in this particular case, will refer to a quantity being ingested, and for those, one needs to refer to the Tolerable Daily Intake (TDI). The TDI is an estimate of the amount of a chemical in air, food or drinking water that can be taken daily over a lifetime without appreciable health risk. TDIs are calculated on the basis of laboratory toxicity data to which uncertainty factors are applied. Migration limits are also applied to estimate how much of a given chemical is released from a matrix or final product, taking into account the main exposure route and relevant body fluid (sweat, gastric fluids, or relevant). The Chemical Safety Assessment and Reporting (Chesar) tool may be used, which provides information for risk assessment derived from chemical dossiers. From this tool, information on consumer and environmental contributing scenarios can be derived (CS). The ConsExpo tool may also be used to calculate exposure of compounds to consumers. A comparative assessment using this tool may be performed with different SSbD solutions.

2.3 Environmental sustainability assessment

For environmental sustainability assessment, the recommended methodology by the EC is the standardised life cycle assessment (LCA) methodology (ISO 14040/44). This comprehensive approach intends to evaluate all the potential environmental impacts of a product or process along its life cycle, thus identifying potential transfer of burdens from one stage to another or from one impact type to another. ISO standards define the following steps to perform a LCA study:

- **Goal and scope definition**, which includes the definition of the context, objectives, audience, system boundaries, functional unit (used to compare equivalent systems providing the same function) and other methodological choices.
- **Life cycle inventory (LCI)**, where all the input and output flows of the studied processes are quantified (foreground data) and complemented with generic data to reflect the upstream and downstream processes (background data, e.g., to model the supply chain of electricity or the treatment processes of waste).
- **Life cycle impact assessment (LCIA)**, where the emissions of pollutants and used natural resources from the LCI step are classified into impact categories and characterized according to their effect and the unit of reference of each impact category (conversion of physical unit from LCI, e.g., mass, to impact unit, e.g., kg CO_2 eq., via a characterization factor, e.g., in kg CO_2 eq./kg reflecting the radiative forcing of the greenhouse gas over 100 years compared to the one of carbon dioxide).
- **Results interpretation**, where the obtained LCA results are analysed depending on the goal of the study and on the quality of the evaluation, e.g., including contribution, gravity, sensitivity or uncertainty analysis, to draw relevant conclusions.

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The application of LCA is iterative, where the practitioner can go back to a previous stage to refine some assumptions, collect more data or test new several scenarios.

Following the recommendations from the EC SSbD framework, besides ISO 14040/44 standards, the LCA will be performed according to the Production Environmental Footprint (PEF) method (EC, 2021), which defines additional rules to increase the replicability and comparability of LCA results. In this project, to model the potential use of secondary materials or the valorisation schemes at the end-of-life (EoL) stage, the Circular Footprint Formula (CFF) will be applied (as recommended by EC, 2021) whenever considered appropriate.

Within ZeroF project, the definition of the goal and scope will depend on each case study, regarding the system boundaries, evaluated scenarios and functional unit (see section 3). Regarding the other aspects, the common objective is to support the design of the new materials, by comparing the environmental impacts of different design alternatives with reference values. The targeted audience is mainly the ZeroF partners who develop the new materials and their processing steps. The evaluation outcomes could nevertheless be communicated externally to support R&I activities for the development of SSbD materials for similar coating systems, as well as policy makers.

LCI data will be collected with project partners (see annex for data collection template) and will be complemented with ecoinvent data (version 3.9.1 or later if available) for background processes (Wernet et al., 2016).

For LCIA step, the PEF method relies on the Environmental Footprint (EF) method (Fazio et al., 2018), which includes a total of 16 impact categories (Table 3), related to toxicity (freshwater ecotoxicity and human toxicity, carcinogenic and non-carcinogenic effects), climate change, pollution (ozone depletion, particulate matter, ionising radiation, photochemical ozone formation, acidification, eutrophication) and resources use (land, water, mineral and metals, and energy carriers).

Table 3: Description of EF impact categories for environmental sustainability evaluation

Impact category	Description	Unit
Human toxicity, cancer	Increased cancer diseases in human population	CTUh[1]
Human toxicity, non-cancer	Increased non-cancer cases in human population	CTUh[1]
Ecotoxicity, freshwater	Potentially affected fraction of aquatic species	CTUe[2]
Climate change	Radiative forcing of GHGs over 100 years	kg CO_2 eq
Ozone depletion	Destructive effects on the stratospheric ozone layer over 100 years	kg CFC-11 eq
Particulate matter	Disease incidence due to particulate matter emissions	disease incidences
Ionizing radiation	Human exposure to radioactive material	kBq U^{235} eq
Photochemical ozone formation	Tropospheric ozone concentration increase due to VOCs oxidation	kg NMVOC eq
Acidification	Critical load exceedance in terrestrial ecosystems due to acidifying substances deposition	molc H^+ eq
Eutrophication, terrestrial	Critical load exceedance in terrestrial ecosystems due to eutrophying substances deposition	mol N eq
Eutrophication, freshwater	Increase of phosphorous concentration in water	kg P eq

Eutrophication, marine	Increase of nitrogen concentration in water	kg N eq
Land use	Index of soil quality	Dimensionless[3]
Water use	Deprivation-weighted water consumption	m^3 water eq. of deprived water
Resource use, minerals and metals	Mineral and metals resource depletion based on use-to-availability ratio	kg Sb eq
Resource use, energy carriers	Fossil resources depletion based on lower heating values	MJ

[1]Comparative toxic unit for humans; [2]Comparative toxic unit for ecosystems; [3]Index reflecting land use impacts from four indicators provided by LANCA model

The characterization of ecotoxicity and human toxicity impacts is based on the consensual method USEtox (Fantke et al., 2017) covering the different steps of the cause-effect chain: fate, exposure and effect. Although the method includes thousands of chemicals (mostly organic substances), not all potentially toxic substances are represented. This is the case of PFAS. For the latter, some authors developed new characterization factors (CFs) to evaluate the impacts of related emissions (the CF is expressed in CTUh/kg emitted or CTUe/kg emitted). Roos et al. (2018) developed freshwater ecotoxicity and human toxicity CFs for 4:2 fluorotelomer alcohol (4:2 FTOH), perfluorohexanoic acid (PFHxA), perfluorooctanoic acid (PFOA) and perfluorobutane sulfonic acid (PFBS). Holmquist et al. (2020) developed freshwater and marine ecotoxicity and human toxicity CFs for PFOA, PFHxa and PFBS with some additional adaptations of the USEtox model (e.g., marine ecotoxicity is normally not included). Differences were observed with the CFs of Roos et al. (2018) due to data choices and different modelling assumptions.

To evaluate the environmental sustainability of a new material/process, criteria should be defined as a reduction of impact category value of X% relative to a reference value. This definition entails the specifications of two aspects: the reference value and the minimum percentage of impact reduction.

Conventionally in LCA, the reference value would be defined as the impacts of the material/process replaced by the new one, fulfilling the same function. In the case of ZeroF, the reference scenario would thus be the replaced PFAS compounds. From the requirements of the funding scheme (HORIZON-CL4-2022-RESILIENCE-01-23), the new materials developed within ZeroF project should generate a reduction of 25 % of environmental impacts compared to the substituted PFAS. This target is nevertheless susceptible to be adapted during the project.

Indeed, for the reference value, the JRC recommends adopting a more ambitious approach to reach not only relative sustainability but the so-called "absolute sustainability" where the impacts of the new developed material comply with the "planetary boundaries". The latter are threshold values for nine environmental aspects, which must not be transgressed to avoid unacceptable environmental change. The definition of the planetary boundaries and their downscaling to a specific process are still under development and no consensual method exist yet, although some works were performed in literature (Bjørn et al., 2020). As a simplified approach, the JRC used a factor of 10 between the current EU production and consumption impacts and the acceptable limits. Further research is needed to consolidate the definition of relevant reference values. In ZeroF, while the replaced PFAS compounds will be firstly used, more ambitious targets aligned with the planetary boundaries will be explored along the project duration.

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Regarding the setting of the percentage in the criteria definition, the JRC does not provide much guidance but only an example with 5 classes, ranging from no improvement to an improvement above 40%, where the material is considered to pass the criteria for an improvement higher than 5%. The authors highlight the need to consider the uncertainty of the assessment to define these classes. This aspect will be investigated in ZeroF project, where the reliability of the LCA will be considered to define the criteria. A key aspect is to avoid that ZeroF materials generate significant additional impacts, where the definition of significant will depend on the evaluation uncertainties. On the contrary, the materials will be considered better than the reference value based on a significant reduction of impacts. The significance could evolve along the project as the quality of data is expected to increase with more representative measurements from the pilot processes.

2.4 Economic sustainability assessment

For an economic sustainability assessment, Life Cycle Costing (LCC) is typically performed following these steps in an iterative manner (similarly to LCA methodology):

- **Goal and scope definition** (same as for LCA, see section 2.3)
- **Data collection**, where the costs for each life cycle stage are collected, including capital costs, operational costs and end of life costs. Assumptions and estimations are often made when the information required is not available or not known with certainty.
- **Life cycle cost assessment**, where the costs are quantified, taking into account factors such as inflation, interest rates. As the costs and benefits do not necessarily occur at the same point in time, a discount rate might be defined and applied to convert all the costs and benefits to a defined reference year and account for the time value of money.
- **Results interpretation and recommendations**, where the obtained LCC results are analysed to evaluate the economic feasibility by showing the economic impact/benefits of the developed solution and draw relevant conclusions. Economic hotspots are identified and recommendations are provided on potential opportunities for further improvement.

In a LCC assessment, the **reference scenario** typically refers to the baseline or standard scenario against which other scenarios or alternatives are compared in terms of cost. As for the LCA in ZeroF project, the reference scenario would thus be the replaced PFAS compounds. PFAS compounds are currently used as they have exceptionally good cost-performance ratio. From the requirements of the funding scheme (HORIZON-CL4-2022-RESILIENCE-01-23), the new materials developed within ZeroF project should be no more than 20% higher in cost of production than current commercial PFAS containing alternatives. This target is nevertheless susceptible to be adapted during the project.

As the LCA will be conducted alongside the LCC, integrating environmental costs and health and safety costs from the LCA into the LCC might provide a more holistic view of the impacts of the developed PFAS alternatives. Depending on the availability and reliability of data, **environmental and health and safety costs** might potentially be calculated for the current commercially PFAS coatings and for the developed alternatives, and included in the LCC assessment.

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The Life Cycle Costing assessment will be conducted by LGI with the aim to evaluate the economic feasibility of the ZeroF solutions. The following cost categories will be taken into account:

- **Capital cost**, including investments in coating machines, acquisition costs, transportation costs, installation costs
- **Operating and maintenance cost**, including basic and auxiliary material consumption, leasing, depreciation, repair costs, staff and labour costs, repairs and technical efficiency maintenance costs, energy consumption costs (boilers, electricity), downtime costs, loss of production costs (decrease in production speed, increased number of interruption), quality problems costs (reduction or lack of water and grease resistance, flame retardancy)
- **End of life cost**, including disposal cost, landfilling cost, recycling cost
- **External cost** (if applicable), including environmental cost, health and safety costs, regulatory compliance costs

Similarly to the LCA, LCC data will be collected with project partners (see section 3.3) and will be complemented with desk research where relevant reference studies sometimes publish the results of previous similar LCC analyses.

The concept of eco-efficiency will be embraced, assessing the ability of the developed coatings to achieve a balance between economic performance and environmental impact. Initially, the eco-efficiency assessment will focus on preliminary data and pertinent reference studies to validate the eco-efficiency potential of the new coatings. In a second stage, the LCC will be revised, incorporating the results of the technical performance evaluation (subtask 6.5.1).

The outcomes of the Life Cycle Costing will contribute to both the exploitation plan and the impact study as part of WP7. Opportunities for further improvement and new customer segments will potentially be identified to help lay the groundwork for the exploitation of project results. If other applications are identified, appropriate reference scenarios may be defined specifically for these new applications at a later stage.

2.5 Social sustainability assessment

Following the requirements of the funding scheme (HORIZON-CL4-2022-RESILIENCE-01-23), the social sustainability assessment will be based on a social acceptance evaluation, considering viewpoints of consumers and other stakeholders. Two models will be combined for characterization of consumer attitudes and social acceptance towards the new coating technology: TAM for technology acceptance and COM-B for behaviour change. The TAM model will bring information regarding how consumers come to accept new technology and how easy they perceive its use. The model considers behavioural intention but doesn’t take stance on possible behaviour change. Hence, the behavioural element will be taken into account with the COM-B model. The COM-B model for behaviour change cites capability (C), opportunity (O), and motivation (M) as three key factors capable of changing behaviour (B). It will be used for studying the awareness and level of understanding regarding sustainability of coated materials, opportunities for carrying out

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choices based on knowledge, and motivation for sustainable behaviour. Additional questions may be included regarding willingness to pay for more sustainable products.

Data will be collected via a quantitative survey study with 1500 respondents from Finland, Luxembourg and greater region, and Spain. This will allow segmentation of consumers based on their level of acceptance and sustainability behaviour. It will also allow comparisons of the attitudes of consumers in Northern, Central and Southern Europe. The data will be shared with Task 7.3 to be used in the design of the Awareness campaign.

Social sustainability is not limited to consumers and hence, other value chain stakeholders will also be included in the discussion. Therefore, up to 30 semi-structured interviews will be carried out with stakeholder representatives. This will ensure the human-centred approach of the project and provide information of other possible incentives and barriers related to the adoption of the technology. We will also explore policy-related issues that may be a barrier, constraint, or a challenge from the viewpoints of the stakeholders.

Possible economic barriers and levers will be addressed together with T7.5 Impact study. After finalizing the task, a final workshop will be arranged with project partners to share the results.

2.6 Integration of SSbD evaluation results

The EC framework defines one cut-off criterion for step 1 regarding the hazard properties of the materials/chemicals, while a score is attributed to the other aspects in steps 2, 3, 4 and 5 depending on the defined criteria. A chemical/material can be considered SSbD if the safety and environmental sustainability are met (socio-economic sustainability is not yet mandatory). When a chemical/material fails a criterion, the latter could be investigated to find solutions for improvement.

In ZeroF, quantitative evaluation of various design alternatives will be performed for the safety, environmental and economic sustainability criteria, while qualitative results on the overall ZeroF concept will be obtained from the social acceptance survey (see section 2.5). The social dimension will thus not be included to support the design choices but could be included as additional qualitative results to understand the acceptance level and barriers of the final ZeroF materials.

In order to rank different design alternatives based on safety, environmental and economic sustainability assessment results, multi-criteria decision analysis (MCDA) can be applied to aggregate all the results and support decisions. Several MCDA techniques exist and can provide different types of outcomes. The JRC (Caldeira et al., 2022a) highlights several requisites and their implications to perform such an assessment. A first key point is the consideration of data quality, which can vary depending on new or existing chemicals/materials and affect the results. Then, both ratings (e.g., poor, good, very good) or numerical values can be used (depending on the defined SSbD criteria). As highlighted previously, the EC aspires to move from a relative evaluation to an absolute one where each chemical or material is evaluated based on its own merits and not compared to other chemicals or materials. Finally, while the hierarchical approach should be respected (safety first), the JRC does not allow for trade-offs between safety and environmental performance, i.e., compensation effects should be minimized. To comply with these requirements, aggregation methods based on IF-THEN rules (e.g., Decision Expert DEX, Dominance based Rouch Set Approach DRSA) or on concordance-discordance voting analysis (e.g., ELECTRE TRI, which proves a good rating if positive results are obtained on sufficient aspects without strong opposition from any of the evaluated aspects) are recommended.

In ZeroF, the targeted TRL at the end of the project for the new developed materials is TRL 5. Intermediate and final SSbD evaluation along the project will still contain significant uncertainties, and more accurate data could be obtained at higher TRL scales. Due to the expected low to medium data quality for the SSbD evaluation, the exclusion of design alternatives because they do not bring significant safety or sustainability benefits is not intended. However, options which are expected to generate significant trade-offs (after considering the range of possible data values) could be excluded. While the results on each aspect of safety, environmental and economic sustainability will be analysed to understand the advantages and disadvantages of ZeroF materials and processes, MCDA techniques will be tested to facilitate the ranking of design alternatives, following the recommendations of the EC. The results will be interpreted based on the data quality, recognising that the SSbD rating will need to be updated during the next phases of the materials development (up to TRL 9).

3 Application of SSbD methodology to ZeroF

This section details the setting for the safety, LCA and LCC assessment of the two ZeroF case studies. These requirements are not necessary for the social acceptance evaluation.

3.1 Packaging

3.1.1 Overall ZeroF process

The project aims to develop silylated cellulose fatty acid ester (CeFAE) to be used as coating material for single-use paper-based packaging. The new coating material is intended to be resistant to water and oil. To fulfil this function, current packaging either used chemical barrier (PFAS) or physical barrier (e.g., plastic film).

The performance of the coating materials will be measured via:

- KIT test to measure the oil/grease resistance
- Cobb test to measure water resistance

In ZeroF, the manufacturing of the CeFAE and its silylation will be investigated, as well as its application on the pulp, with different coating processes, forming and drying. The impacts on the use and disposal are also analysed, in particular the recyclability of the new packaging material (e.g., via mechanical disintegration and reuse in air-forming).

3.1.2 State-of-the-art regarding safety and sustainability performances

Rising concerns with the environmental impact of disposable packaging materials and associated waste led to the definition of stricter requirements on the use of disposable fossil-based packaging (Directive 2019/904) and for material recovery after packaging disposal (Directive 2018/852). In this context, fibre-based packaging material is seen as a valuable alternative given that it is made from renewable sources and has the highest recycling rate amongst the different types of packaging materials in the European Union (Svensson 2021).

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While not any renewable source can be considered environmentally better than a fossil based one, cellulose-based packaging is a promising one since moulded pulp is obtained only from inedible fibrous wastes such as stalks, leaves and not from primary crops grown and transported specifically to manufacture the packaging (Semple et al. 2022).

Moulded pulp packaging can be obtained either via a wet moulding or a dry moulding process. In wet moulding, pulp is mixed with water to form a slurry which is then made into a packaging shape via thermoforming, while in dry moulding pulp fibers are laid into a network using air streams, and then pressing and shaping the fibers layer into the packaging shape using a 3D mould (Svensson 2021). To ensure that the packaging does not break down due to water, temperature, grease and vapour, a barrier addition is needed. A barrier can be physical when an additional layer of impermeable material (i.e., plastic) is added to the fibre layer, and chemical if an additive is added in the pulp or applied on the surface to be absorbed directly into the fibres. Given their oil and water repellent properties, PFAS have been widely used as additives to make food contact materials impermeable to grease and water since the 1950’s (Larsson 2022).

Due to their stability and persistency, PFAS have become ubiquitous substances in the environment and have bioaccumulated in animals and plants. Moreover, due to their amphiphilic properties (i.e., possessing both hydrophilic and lipophilic properties), they can easily migrate into food oils making the food contained into PFAS coated packaging a dominant contamination route for humans (Larsson 2022; Semple et al. 2022).

On the other hand, cellulose fibres are molecular and chemically identical to celluloses already authorized and used in food for decades (FDA, 2018). Studies over-estimating human intake of cellulose fibres did not conclude on significant adverse effects in mammals (oral exposure route), studies included *in vitro* genotoxicity assessment (OECD 487 in vitro micronucleus test) and a 90-day OECD TG 408 study (Ong et al., 2020). As a result, the Joint FAO/WHO Committee on Food Additives (JECFA) assigned an acceptable daily intake of celluloses as “not specified,” which is assigned to substances of very low toxicity (JECFA, 1975).

In literature, LCA studies of takeaway food containers made with cellulose based materials (i.e., moulded pulp packaging) are extremely limited. Of the few that are available in the scientific literature, only Gihring (2022) included the modelling of a water and grease resistant component. The latter is assumed to be a mix of starch and bentonite clay based on Khairuddin et al. (2019). No LCA studies were found on the modelling of PFAS for packaging application.

3.1.3 System boundaries for SSbD evaluation

Following the EC recommendations for SSbD evaluation, the various steps of the life cycle of the new coating material for packaging are included (Figure 2):

- Synthesis of the new coating material, i.e., acylation and silylation process for CeFAE
- Coating and finishing processes to obtain the final product (coated packaging), including coating preparation, drying, forming and printing
- Transport and use of the coated packaging
- Disposal of the coated packaging

For the safety assessment, the hazard properties of the materials and reagents will be first assessed (step 1), and then the risk will be evaluated based on the emissions during the production and further processing steps (including synthesis, coating, finishing, and disposal) for the step 2 of the framework, while the emissions during use will be considered for the step 3. Following the JRC stepwise framework substances falling into the SVHC may not be used to achieve the CSS goals, if required, they may be used under the "essential use" concept (EC, 2023).

For the LCA and LCC evaluation, other input and output flows will be considered, in particular the impacts of raw materials, energy, additives, transport and waste treatment. The environmental impacts of the infrastructures will be neglected for the LCA. However, the capital costs and labour costs will be included for the LCC.

Flows or processes that are observed to have a negligible effect on the results or are estimated not to be affected by the new coating material could be excluded for the system boundaries, e.g., the supply of fluff pulp for the packaging production.

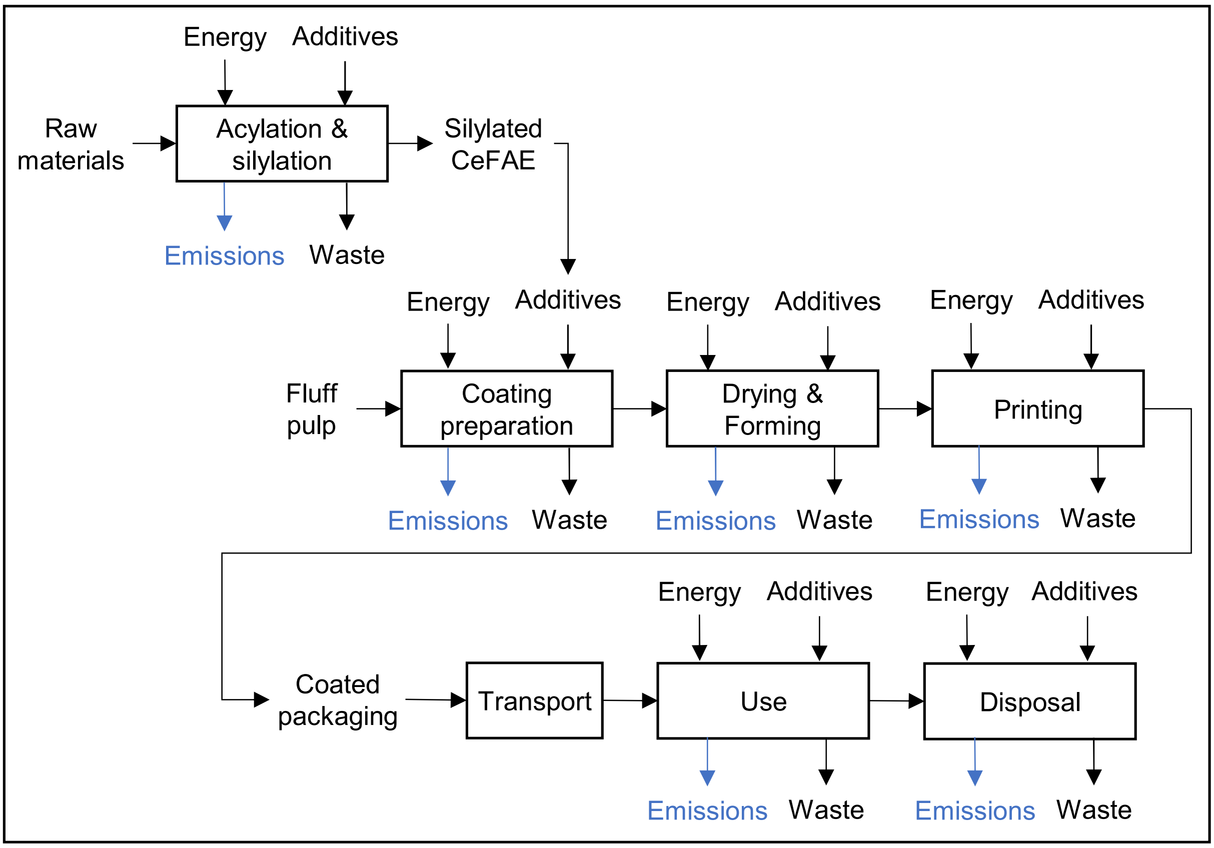

Figure 2: System boundaries for the SSbD evaluation of the packaging application. Flows in black will be included for the LCA and LCC while flows in blue will be also considered for the safety assessment.

As mentioned in the section 3.1.1, the first reference value used to evaluate the environmental and economic benefits or disadvantages of the new coating material will be the one of the common PFAS used for paper-based packaging coating, i.e., TG-8111. Further targets, aligned with the planetary boundaries concept, will be considered as alternative reference values for the LCA study, following EC recommendations.

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To compare scenarios on a common basis, LCA and LCC evaluation will consider the following functional unit: keep 1 m^2 of paper-based single-use packaging resistant to water and oil in Europe.

3.1.4 Design alternatives to be investigated

Within ZeroF project, different design alternatives of the new CeFAE-based coating material will be investigated. To support these design choices beyond technical criteria, intermediate SSbD evaluation will be performed on the following aspects:

- Different starting materials (polysaccharides) for CeFAE synthesis
- Different solvents for CeFAE synthesis
- Operating conditions for CeFAE synthesis
- Alternative coating processes (dry coating, liquid spray, foam coating)

The consequences of these design alternatives on the rest of the life cycle will be considered. This will be done by continuous exchanges with the materials developers and on data collection file, adapted to collect data for several scenarios along the project (see section 3.3).

3.2 Textile

3.2.1 Overall ZeroF process

Within ZeroF project, a new silicone-based organic-inorganic hybrid coating (ORMOCER®) will be developed, as well as its coupling with the CeFAE material (see section 3.1) to improve the coating material performances for textile application.

To protect textiles from water and oil, PFAS with six carbons in the chain (C6) are usually applied on the fabric. Current PFAS-free products for textile finishing lack oil repellency properties. With the new ZeroF material, the same water repellence of C6 is targeted while additional oil repellence is intended to be provided. The new ZeroF materials also aim to provide safer environmental alternatives to the current use of PFAS.

The performances of the coated materials will be measured via standardised methods for water and oil repellency. Water repellency will be tested according to UNE EN ISO 4920 or AATCC 22, and a minimum target of 4 out of 5 is expected. For oil repellency, UNE EN ISO 14419 or AATCC 118 will be followed, with a minimum target of 4 out of 8. The repellent properties will also be tested after washing in order to determine the coating durability. Abrasion resistance (ISO 12947-2) and other properties, such as flexibility or comfortability, could be also tested.

The ORMOCER® synthesis and its coupling with silica particles will be investigated. The coating and finishing processes will be also analysed, in particular the need for a potential plasma pre-treatment, different coating processes and the final drying and curing of the textile. As for the packaging case study, the use and disposal impacts will be included, where the recyclability of the new textile material will be analysed.

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3.2.2 State-of-the-art regarding safety and sustainability performances

Durable water repellent substances (DWRs) are chemical substances that are applied during the finishing step of textile manufacturing to provide liquid repellence (water and oil) to the fabric. Amongst the most used DWRs are PFAS. These molecules migrate in the environment either from direct emissions during their manufacturing and use phases during textile production, but also during the life cycle of the textile, diffused in the environment as part of the microfibers lost due to usage and washing (Shellenberger et al. 2019a). The degradation in the environment of PFAS molecules, leads to the production of perfluoroalkyl acids (PFAAs) which are chemically highly stable, making them extremely persistent in the environment and capable to bioaccumulate. Consequently, the rising exposure from wildlife and humans to these ubiquitous substances has led to increasing concerns of toxic effects on ecosystems and humans alike (eco-toxicity) (Schellenberger 2019b). Following these concerns, the European Union (EU) has set stringent limits to their use with a maximum concentration of 1μg/m^2 in textile fabric and most of the PFAS have been classified as persistent, bioccumulative and toxic substances under the Stockholm Convention on Persistent Organic Pollutants.

In the scientific literature, the use of PFAS in textile manufacturing have been seldomly included in LCA studies and are mainly limited to the evaluation of outdoor clothing fabric. The LCA evaluation of textile coating with PFAS raises two main challenges. First, the modelling of the PFAS production impacts raises challenges due to the difficulty to access composition and process information (confidentiality issues) (Roos et al. 2019). Authors used publicly available information and proxy data, which increases the uncertainty of the assessment. Then, the lack of CF for PFAS to characterise toxicity-related impacts in LCA underestimates the toxicity impact of a textile product coating with PFAS . The definition of the fate (depending among others on its persistence), exposure levels and toxicity effects of a chemical substance or its degradation products are fundamental for their evaluation during the life cycle impact assessment and are used to derive CF (Holmquist et al. 2020). If the CFs of PFAS are excluded due to a lack of data, the LCA results thus only represent characterised toxic substances, e.g., due to emissions from the supply chain of raw materials (Roos et al. 2015).

The first identified LCA study on PFAS used for textile is from Gore & Associates (2013). The authors compared the environmental impacts of a waterproof jacket, with a C8, short-chain fluoropolymer or with a fluorine-free alternative DWR. The toxicity-related impacts of PFAS emissions were not included (no CF). No significant differences were found between scenarios, but the washing impacts were assumed higher for the fluorine-free jacket.

As highlighted in section 2.3, two studies developed new CF to characterize the toxicity-related impacts of PFAS in LCA, Roos et al. (2018) and Holmquist et al. (2020).

The CFs developed by Roos et al. (2018) were used in the LCA study of Fierro and Martinez (2018). This work evaluated the environmental impacts of DWR alternatives for the finishing of 100 m^2 of fabric (DWR application, drying and curing processes). The further use and disposal phases are excluded from the study. The studied DWR included C8 and C6 fluorinated compounds, perfluorosilicone, silicone, dendrimer and paraffin. The modelling of PFAS manufacturing was based on publicly available data, with significant assumptions, and process emissions were based on the "Default worst-case release factors" from the

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European Chemical Agency (ECHA, 2016). The authors found lower environmental impacts for the non-fluoro alternatives, mainly due to lower production impacts (relatively small impacts of the drying and curing process). The high impacts of PFAS alternatives are mostly due the human toxicity effects (PFAS emissions) and ozone depletion effects (release of CFCs during the production of tetrafluoroethylene used as precursor for PFAS).

In Holmquist et al. (2020), the developed CFs were applied to an illustrative case study to compare the impacts of producing two types of surgical protective drapes, one coated with a PFAS and the other one coated with a plastic film. The PFAS was assumed to be C6 PFAS, whose production was modelled based on an US dataset from GaBi database, and related emissions of degradation products during the PFAS manufacturing and textile finishing process were estimated by the authors. Other life cycle steps are not included in the study. The results showed higher impacts of the plastic-coated drape than the PFAS one in terms of carbon footprint and ecotoxicity, but variable human toxicity results (non-carcinogenic effects) depending on the data used to model the emissions and CF of PFAS. Indeed, several assumptions were used to model these impacts and all of them led to lower impacts of the PFAS-coated drape except if extrapolated human epidemiological data were used to model the effect factor for the CF calculation (and not rodent data), regardless of the emissions scenario.

The CFs of Holmquist et al. (2020) were also used in a more comprehensive assessment (Holmquist et al., 2021) for the comparison of the environmental impacts of different DWR alternatives for a shell jacket. The whole life cycle of the jacket was considered, including the manufacturing of the jacket and of the DWR, the finishing process, the use and disposal of the jacket. The studied DWR are C8, C6 and C4 PFAS, a silicone-based DWR, a hydrocarbon-based wax and a non-fluorinated DWR based on hyperbranched polymers. Data available in literature and database (GaBi dataset for PFAS, as in Holmquist et al., 2020) were used to model the life cycle inventory, while several emission scenarios were tested. The only critical difference between the DWR alternatives concern the human toxicity impacts (non-carcinogenic), for which non-fluorinated DWR have less than 0.1% of C8 toxicity, thanks to avoided PFAS emissions (mainly generated during use phase), which greatly influence this factor. However, the carcinogenic human toxicity, ecotoxicity and climate change impacts are mainly influenced by the textile manufacturing and the energy consumption of the finishing process, which leads to no significant differences between DWR alternatives. As for Holmquist et al. (2020), the non-carcinogenic benefits of non-fluorinated DWR are not visible if rodent data are used to model the effect factor within CF calculation for PFAS.

This literature review showed different conclusions based on the studies. Depending on the modelling of the production impacts of DWR, the latter had significant contribution to LCA results or not (increasing the role of finishing process), thus influencing the conclusions. Besides this, the authors who included the CF for PFAS highlighted potential benefits on non-carcinogenic human toxicity thanks to the use of PFAS alternatives. This highlights the necessity to collect good quality data for the DWR production and include the effects of the PFAS emissions along the product life cycle to obtain reliable comparative LCA results.

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3.2.3 System boundaries for SSbD evaluation

As for the packaging application, the entire life cycle of the new coating material for textile are considered (Figure 3):

- Synthesis of the new coating material (ORMOCER® with the silica coupling)
- Coating and finishing processes to obtain the final product (coated textile), including formulation preparation and application, drying and curing
- Transport and installation of the coated textile
- Use of the coated textile
- Disposal of the coated textile

The safety assessment will first focus on the hazard properties of the used materials (step 1), while the safety risks will be evaluated depending on the emissions during the production and processing steps (step 2), as well as during the use phase (step 3). Step 2 will be based on ECHA's use maps and semi-quantitative control banding tools, whereas step 3 will use tools such as ConsExpo.

The other energy and material flows will be included for the LCA and LCC evaluation. As for the packaging case, the infrastructures impacts will be neglected for the LCA, while the capital and labour costs will be considered for the LCC.

Flows or processes that are observed to have a negligible effect on the results or are estimated not to be affected by the new coating material could be excluded for the system boundaries, e.g., the transport and installation of the coated textile.

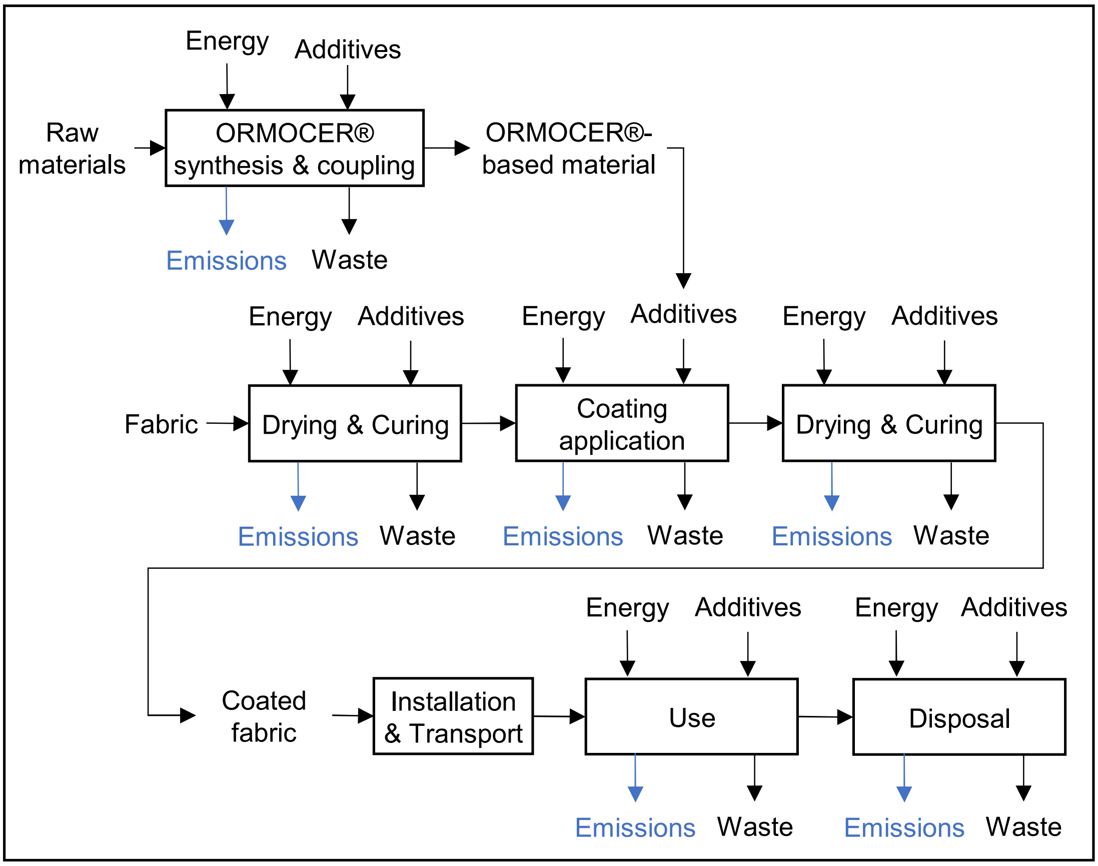

Figure 3: System boundaries for the SSbD evaluation of the textile application. Flows in black will be included for the LCA and LCC while flows in blue will be also considered for the safety assessment.

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As mentioned in the section 3.2.1., the reference scenario to evaluate the environmental and economic impacts of the new coating material will be the use of PFAS C6 to coat fabric. More ambitious targets will be investigated during the project (for an absolute sustainability assessment, see section 2.3).

The same functional unit should be considered the ZeroF and reference scenarios for the LCA and LCC studies. As highlighted in section 3.2.1, the ZeroF material intends to bring additional functionality in terms of oil repellence. This could not be translated into the functional unit since no material can nowadays provide this function but will be considered via the modelling of the impacts, in particular regarding the use phase (e.g., longer lifetime or less washing). The functional unit is thus defined as followed: keep 1 m^2 of upholstery textile resistant to water, oil and abrasion for one year in Europe.

3.2.4 Design alternatives to be investigated

To support the design choices regarding the development of the new coating material for textile application, intermediate SSbD results will be provided for the following alternatives:

- Different materials for the inorganic and organic preforming for ORMOCER® synthesis
- Different solvents for coating material synthesis
- Operating conditions for coating material synthesis
- Use of plasma pre-treatment or not
- Alternative coating processes (padding, exhaustion)

As for the packaging case study, the consequences of the design choices on other life cycle steps will be evaluated via direct exchanges with the materials developers and continuous data collection.

3.3 Required data for the evaluation

A data collection template was developed to be able to regularly collect the necessary information to support the material development via SSbD (one file for each application, i.e., packaging and textile, with similar structure).

The latter is divided into different tables, one for each step of the life cycle: i) Manufacturing of coating material, ii) Coating and finishing processes, iii) Distribution, use and disposal (further divided into sub-processes). For each sub-process, the material inputs, energy inputs, products, waste, emissions, as well as capital and labour data are intended to be collected. For each of this flow, the following information are required (see Figure 4):

- **Flow information:** name and specifications of the flow (e.g., electricity from the grid, solid waste to incineration)
- **Safety information:** CAS number and the safety data sheet link (if available)
- **Quantity information:** amount of the flow with the respective unit, with additional columns to be filled if several design alternatives exist and affect the quantity value
- **Cost and supplier information:** unit price, supplier(s) name and respective location

- **Data source information:** name of the data provider, date and any additional information regarding the source of data (e.g., measurement, estimation, literature). This information will be used to evaluate the data quality of the evaluation.

Flow information		Safety information		Quantity information				Cost & supplier information			Data source information		
Name	Description	CAS number	MSDS?	Unit	Baseline value	Altern. #1	Altern. #2	Unit price (€)	Supplier(s)	Location	Partner	Date	Comments (data source, quality...)
1. Manufacturing of coating material													
1.1. Material synthesis (option 1)													
1.2. Material synthesis (option 2)													
Material inputs													
Chemicals name	Chemical function/type			kg									
Chemicals name	Chemical function/type			kg									
Chemicals name	Chemical function/type			kg									
Energy inputs													
Electricity	Please specify source	[redacted]		kWh									
Heat	Please specify source			MJ									
Water	Please specify source			m3									
Products													
ORMOCER-coating system	**Main product**	[redacted]		**kg**									
Solid/liquid waste													
Waste type	Please specify disposal mode	[redacted]		kg									
Emissions of pollutants													
Pollutant name	Emissions to air	[redacted]		kg				[redacted]					
Pollutant name	Emissions to soil			kg									
Pollutant name	Emissions to water			kg									
Capital and labour													
Purchase and acquisition	Please specify product	[redacted]											
Transportation and installation	Please specify product												
Labour	Labour cost			hour									
2. Coating & finishing processes													
2.1. Plasma pre-treatment													
2.2. Padding coating alternative													
2.3. Exhaustion coating alternative													
2.4. Drying and curing method													
3. Use & disposal													
3.1. Distribution													
3.2. Use													
3.3. Textile disposal													

Figure 4: Print screen of the SSbD data collection file (example for textile application, similar file used for packaging application).

Regarding safety and to cover for step 1, a colour-coded excel was developed to discern to which of the three categories reagents belong to (most harmful substances, hazardous substances and other substances). To facilitate selection of chemicals, collected safety data was colour-coded as follows: red (most harmful substances), pink (hazardous substances), green (other substance classes or not classified to corresponding end point), yellow (no data) as shown in Figure 5.

Materials Information					Human Health hazards																Environment		
Name	CAS	Partner	MSDS	Comments	Carcinogenicity	Mutagenicity	ReprTox	End dis (human)	Respiratory sensitization	STOT-RE	Skin sens	Acute tox (oral)	Acute Tox (dermal)	Acute Tox (inh)	Skin corr	Skin irr	Eye damage	Eye irr	Aspiration hazard	STOT-SE	PBT/vPvB	PMT/vPvM	End dis (env)
[redacted]					miss	miss	miss			miss		miss	not clas	miss	miss			cat 2	miss	cat 3	not	not	miss
[redacted]					miss	cat 2	cat 1	not class		cat 1	cat 1	cat ?	cat?	miss	not class			cat 2	miss	cat 1	not	not	not
[redacted]					cat 2	not clas	miss	Not cla	Not cla	miss	not clas	cat 2		cat ?	not class			cat 2	miss	cat 3	not	not	not
[redacted]					miss	cat ?	miss	not clas	not clas	miss	not clas	cat 4	miss		cat 1	cat 2	cat 1	cat 2	miss	cat 3	not	not	not
[redacted]					miss	not clas	miss	Not cla	cat 1	miss	cat 1	cat 1	cat 1	cat 1	cat 1	cat 2	cat 1	cat 1	miss	cat 2	not	not	not
[redacted]																							
[redacted]					miss	miss	miss	not clas	miss	miss	miss	miss	miss	miss	miss	cat 2	miss	cat 2	miss	cat 3	not	not	not
[redacted]					miss	miss	miss	not clas	miss	miss	miss	miss	miss	miss	miss	cat 2	miss	cat 2	miss	cat 3	not	not	
[redacted]																							
[redacted]					not clas	not clas	cat 2	not clas	not clas	cat 2	not clas	cat?	miss	cat?	cat?	cat 2	cat?	cat 2	cat 1	cat 3	not	not	not
[redacted]					miss	miss	evidenc	not clas	miss	cat 2	miss	cat 4	miss	cat 4	miss	cat 2	miss	miss	cat 1 *	cat 3	not	not	not
[redacted]					miss	miss	miss	not clas	miss	miss	miss	miss	miss	miss	evidenc	vidence	miss	cat 2	miss	cat 3	not	not	not
[redacted]					miss	miss	miss	not clas	miss	not clas	miss	miss	miss	miss	slight	slight	slight	slight	miss	not clas	not	not	not

Figure 5: Evaluation of chemicals in ZeroF (chemicals name and characteristics hidden due to confidentiality issues). Relevant end points (top) are collected per chemical reagent (left of table)

4 Conclusion

Within ZeroF project, safety and sustainability criteria will be used to steer the design of the new developed materials and processes and enhance their benefits, following the EC SSbD framework. Besides the potential application of design principles such as waste recovery or

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energy efficiency, the safety and sustainability performances of the new materials and the design alternatives will be evaluated with a life cycle perspective following the JRC stepwise approach.

The three safety steps will be performed using publicly available data, but also filling data gaps thanks to experimental hazard testing and the use of computational models. For environmental sustainability (step 4), LCA methodology will be applied following the PEF method. This evaluation intends to tackle potential missing characterization factors and investigates approaches to define criteria considering the planetary boundaries and the modelling uncertainties. The economic sustainability assessment in step 5 will be based on LCC methodology, where the same settings than for the LCA will be applied for a harmonized assessment. These assessments will be performed in an iterative manner along the project to support design choices, where several aggregation approaches will be tested to rank the possible options. Besides this, the social acceptance of the ZeroF materials will be evaluated based on surveys and interviews. However, the related results will not be used to steer design choices (only one final evaluation).

To apply the SSbD methodology to the materials developed for packaging and textile coating, several modelling choices were made. First, the life cycle approach is applied but potential processes or flows which do not affect the results could be excluded (e.g., transport). The life cycle steps can be divided into coating material synthesis, coating and finishing processes, and use and disposal of the final product. For the LCA and LCC evaluation, the reference flow of 1 m^2 of coated product (packaging or textile) will be used while the functional unit additionally includes the targeted performances (water and oil repellence). The reference scenario considered will be the common PFAS compound used in each of the application, but more ambitious targets will be defined along the project to move towards an "absolute" assessment. The investigated design alternatives concern the use of different raw materials, additives or operating conditions for the material synthesis but also the type of coating process. To efficiently collect data for the SSbD evaluation, a common Excel file was prepared to collect the necessary data for the safety, environmental and economic sustainability assessment, keeping track of data quality.

The SSbD methodology is subjected to changes and potential updates during the project lifetime, since the EC framework is expected to be revised in 2025, after having collected feedback from the SSbD case studies and R&D projects. The ZeroF consortium is participating in the revision process, by joining the Stakeholder workshops and consultations, in order to provide feedback through the ZeroF case studies and their ongoing application. The consortium will follow the future developments on European level and synchronise the ZeroF SSbD framework as deemed necessary.

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