Safe-, sUstainable- and Recyclable-by design Polymeric systems
A guidance towardS next generation of plasticS

Start date of the project: 01/06/2022
Duration 42 months

Deliverable D4.1

Polymeric material specific SSRbD criteria and scoring strategy

Work Package	**4**	Development and use of SSRbD Assessment tools, methods and guidance
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Nature of the deliverable		
R	Report, document	☒
DEC	Websites, patents filing, press & media actions, videos, etc.	☐
DMP	Data Management Plan	☐

Dissemination Level		
PU	Public, fully open	☒
SEN	Sensitive, Restricted to a group specified by the consortium under conditions set out in grant agreement	☐

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Executive summary

A review of previous and on-going Safe, Sustainable and Recyclable by Design (SSRbD) initiatives was made including monitoring policy developments such as the general framework developed by the EU Commission for framework for Safe and Sustainable by Design (SSbD) criteria which takes into account the entire life cycle. The operationalization of the SSRbD criteria for polymeric materials was aligned to these ongoing international initiatives and internally with the SURPASS consortia. A series of internal workshops were organized during T4.1 meetings to brainstorm on how to operationalize the proposed SSbD framework from the EC to polymeric material specific SSRbD in a co-creation process involving participants from WP2 & WP3 and risk assessors, toxicologists, hygienists, eco-design and sustainable development experts and regulators. The translation of the EC JRC framework to fit SURPASS project was performed through the development of a holistic life cycle thinking. The Safe-Sustainable-and-Recyclable-by-Design Approach consists of the following steps:

1. The identification of criticality, toxicity, environmental, social, circularity, functionality and economic impacts in a life cycle thinking perspective per case study
2. The development of Safe-Sustainable-and-Recyclable-by-Design strategies
3. Verification of Safe-Sustainable-and-Recyclable-by-Design strategies to ensure they lead to safer and more sustainable alternatives

This first 2 steps are being applied to the 3 cases studies (***Building sector, Case Study CS#1:*** New recyclable-by-design bio-sourced polyurethane (PU) to replace PVC (Polyvinyl Chloride) as insulating material for window frames; ***Transport sector, Case Study CS#2:*** Fire resistant, intrinsically recyclable epoxy-vitrimer materials for sustainable composites to replace metal for train body; ***Packaging sector, Case Study CS#3:*** Recyclable MultiNanoLayered (MNL) films to replace multi-layer films for packaging with drastically reduced concentrations of compatibilizers). These include the identification of criticality, toxicity, environmental, social, circularity, functionality and economic impacts in a life cycle thinking perspective per case study. For each of the case studies, the biggest safety & sustainability challenges, and the development of SSRbD strategies. Ongoing work is on the optimization of the SSRbD strategies and Step 3, which is the verification that these are safer and more sustainable alternatives.

A communication and visualization (qualitative scoring) dashboard is proposed consisting of 1. Functionality, 2. Safety, 3. Environmental Sustainability, 4. Economical Sustainability, and 5. Social Sustainability. These will be translated to KPIs that can guide SMEs into identifying safety and sustainability hotspots and development of impact-driven SSRbD strategies.

Finally, in terms of internal organization, an interdisciplinary group for case study group encompassing partners from release and exposure (T4.2), Hazard, (T4.3), Health and environmental impact (T4.4) and Life cycle costing (T4.5) was developed and is actively supporting the further development of the SURPASS SSRbD approach.

Deliverable Review*

	Reviewer #1: .Simon Clavaguera............			Reviewer #2:		
	Answer	**Comments**	**Type***	**Answer**	**Comments**	**Type****
1. Is the deliverable in accordance with						
- the Description of Work?	☒ Yes ☐ No		☐ M ☐ m ☐ a	☐ Yes ☐ No		☐ M ☐ m ☐ a
- the objectives of the WP and specific tasks?	☒ Yes ☐ No		☐ M ☐ m ☐ a	☐ Yes ☐ No		☐ M ☐ m ☐ a
2. Is the quality of the deliverable in a status						
- that allows it to be sent to European Commission?	☒ Yes ☐ No		☐ M ☐ m ☐ a	☐ Yes ☐ No		☐ M ☐ m ☐ a
- that needs improvement of the writing by the responsible of the section?	☐ Yes ☒ No		☐ M ☐ m ☐ a	☐ Yes ☐ No		☐ M ☐ m ☐ a
- that needs further work by the Partners responsible for the deliverable?	☐ Yes ☒ No		☐ M ☐ m ☐ a	☐ Yes ☐ No		☐ M ☐ m ☐ a

*To be removed prior to be sent to the European Commission

**Type of comments: M = Major comment ; m = minor comment ; a = advice

List of acronyms

3R	Recyclable, Reprocessable and Repairable
ADP	Abiotic resource depletion
AE	Accumulated Exceedance
APP	Ammonium polyphosphate
ATH	Aluminium trioxide
CLP	Classification, Labelling and Packaging [Regulation (EC) nº 1272/2008]
CMR	Carcinogenic, Mutagenic and Toxic for Reproduction
CS	Case Study
CSR	Corporate Social Responsibility
CSS	Chemical Strategy for Sustainability
CTU_e	Comparative Toxic Unit for humans
CTU_h	Comparative Toxic Unit for ecosystems
DMTA	Dynamic Thermal Mechanical Analysis
DSC	Differential Scanning Calorimetry
EC	European Commission
ECHA	European Chemical Agency
ED	Endocrine Disrupting
ESPR	Ecodesign for Sustainable Products Regulation
EU	European Union
EU-CSS	EU- Chemical Strategy for Sustainability
EvOH	Ethylene and Vinyl Alcohol copolymer
FR	Flame Retardant
FRPC	Fibre-reinforced plastic composite
FST	Fire, Smoke and Toxic
FTIR	Fourier transform infrared
GWP	Global Warming Potential
HDPE	High Density Polyethylene
IAS	Intended Added Substance
JRC	Joint Research Centre
KPI	Key Performance Indicator
LCA	Life Cycle Assessment
LCC	Life Cycle Costing
LCI	Life Cycle Inventory
LCS	Life Cycle Stage
LCSA	Life Cycle Sustainability Assessment
LDPE	Low Density Polyethylene
MCI	Material Circularity Indicator
MNL	MultiNanoLayered
NIAS	Non-Intended Added Substance
ODP	Ozone Depletion Potential
OSHA	Occupational Safety and Health Administration (United States)
PA	Polyamide
PBT	Persistent, Bioaccumulative and Toxic
PEF	Product Environmental Footprint
PE-g-MA	Polyethylene grafted with maleic anhydride
PET	Polyethylene Terephthalate
PM	Particulate Matter
PMT	Persistent, Mobile and Toxic

PP	Polypropylene
PU	Polyurethane
PVC	Polyvinyl Chloride
QSAR	Quantitative Structure-Activity Relationship
REACH	Registration, Evaluation, Authorisation and restriction of Chemicals [Regulation (EC) nº 1907/2006]
REPA	Resource and Environmental Profile Analysis
RTM	Resin Transfer Moulding
SDG	Sustainable Development Goals
SDS	Safety Data Sheet
SpERC	Specific Environmental Release Category
SPI	Sustainable Product Initiative and Regulation
SSbD	Safe-and-Sustainable-by-Design
SSRbD	Safe-, Sustainable-, and Recyclable-by-Design
STOT-RE	Specific Targeted Organ Toxicity – Repeated Exposure
STOT-SE	Specific Targeted Organ Toxicity – Single Exposure
SVHC	Substances of Very High Concern
Tg	Glass transition temperature
TGA	Thermal Gravimetric Analysis
TRL	Technology Readiness Level
VOC	Volatile Organic Compound
vPvB	Very Persistant, very Bioaccumulative
vPvM	Very Persistant, very Mobile
VRE	Value-based Resources Efficiency indicator
WP	Work Package

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1 Introduction

Plastic waste outlives us on this planet as they take centuries to break down. Endocrine disruption, land, air, and water pollution are only some of the adverse effects of plastic waste on public and environmental health. Still, 70% of plastic waste collected in Europe is landfilled or incinerated.

The main objective of SURPASS project is to lead by example in the transition towards more Safe, Sustainable, and Recyclable by Design (SSRbD) polymeric materials. Therefore, we develop SSRbD alternatives with no potentially hazardous additives through industrially relevant case studies targeting the three sectors representing 70% of the European plastic demand:

- Building sector _ Case Study CS#1: New recyclable-by-design bio-sourced polyurethane (PU) to replace PVC as insulating material for window frames.
- Transport sector _ Case Study CS#2: Fire resistant intrinsically recyclable epoxy-vitrimer materials for sustainable composites to replace metal for train body.
- Packaging sector _ Case Study CS#3: Recyclable MultiNanoLayered (MNL) films to replace multi-layer films for packaging with drastically reduced concentrations of compatibilizers.

In particular, WP4 will operationalize sets of aspects, adapt and develop methods, and build user-friendly scoring strategies to assess the three domains of sustainability of polymers developed in WP2 & 3. Inventories of physicochemical properties of additives, side products, processing aids, degradation products and contaminants detected in plastics will be compiled and their link to functionality and human and environmental toxicity will be investigated.

This deliverable D4.1 will be focused on the development of a practical strategy that is aligned to the JRC framework for SSbD criteria for polymeric materials in the three case studies (building sector, transport sector and packaging sector).

2 Description of the tasks

Task 4.1: Scoping for policy alignment and process structuration to operationalize and evaluate polymeric material specific SSRbD criteria

RIVM, LEITAT and CEA will make a review of previous and on-going SSRbD initiatives including monitoring policy developments such as the general framework developed by the EU Commission for framework for SSbD criteria which takes into account the entire life cycle. The operationalization of the SSRbD criteria for polymeric materials will be aligned to ongoing international initiatives (see Section 1.2.2 - RIVM, LEITAT) and internally with the SURPASS consortia. A series of internal workshops, moderated by CEA and RIVM, will be organized at the beginning of the project to operationalize the proposed SSbD criteria from the EC to polymeric material specific SSRbD in a cocreation process involving participants from WP2 & WP3 and risk assessors, toxicologists, hygienists, eco-design and sustainable development experts and regulators. Results of these workshops will help refining the scope of the assessments (release scenarios, toxicological endpoints, impact categories, system boundaries, functional unit) and promote the WP4 cross-fertilization. Conclusions will be shared with the consortium and forwarded to T5.1.

An inventory of the tools and methods to be used in further tasks and the assessment of their interoperability will be made in order to have a holistic vision of the product's sustainability impacts looking for common key parameters needed to establish a SSRbD strategy (CEA, LEITAT, RIVM).

3 EC JRC SSbD Framework

The SSbD concept may be considered as the identification of sustainability (safety, risks concerning humans and the environment, environmental, social and/or economic impacts) hotspots at an early phase of the innovation and product development process in order to minimize potential hazard(s) and/or exposure [3], and to maximize sustainability. A first description of the SSbD concept can be found in the EU - Chemical Strategy for Sustainability (EU-CSS): "safe and sustainable-by-design can be defined as a pre-market approach to chemicals that focuses on providing a function (or service), while avoiding volumes and chemical properties that may be harmful to human health or the environment, in particular groups of chemicals likely to be (eco) toxic, persistent, bio-accumulative or mobile. Overall sustainability should be ensured by minimizing the environmental footprint of chemicals in particular on climate change, resource use, ecosystems and biodiversity from a life cycle perspective" [4].

The EC Joint Research Centre (JRC) has developed a framework for SSbD criteria where a two-phase approach is recommended (Figure 1): a (re)-design phase in which guiding principles are proposed to support the design of chemicals and materials and in the second phase a step-wise hierarchical approach to address chemical safety, direct toxicological/ecotoxicological impact, and aspects of environmental sustainability [5]. The **JRC Framework defines a SSbD criterion as 'an aspect with an assessment method and a minimum threshold or target values (on which a decision may be based)**' [5].

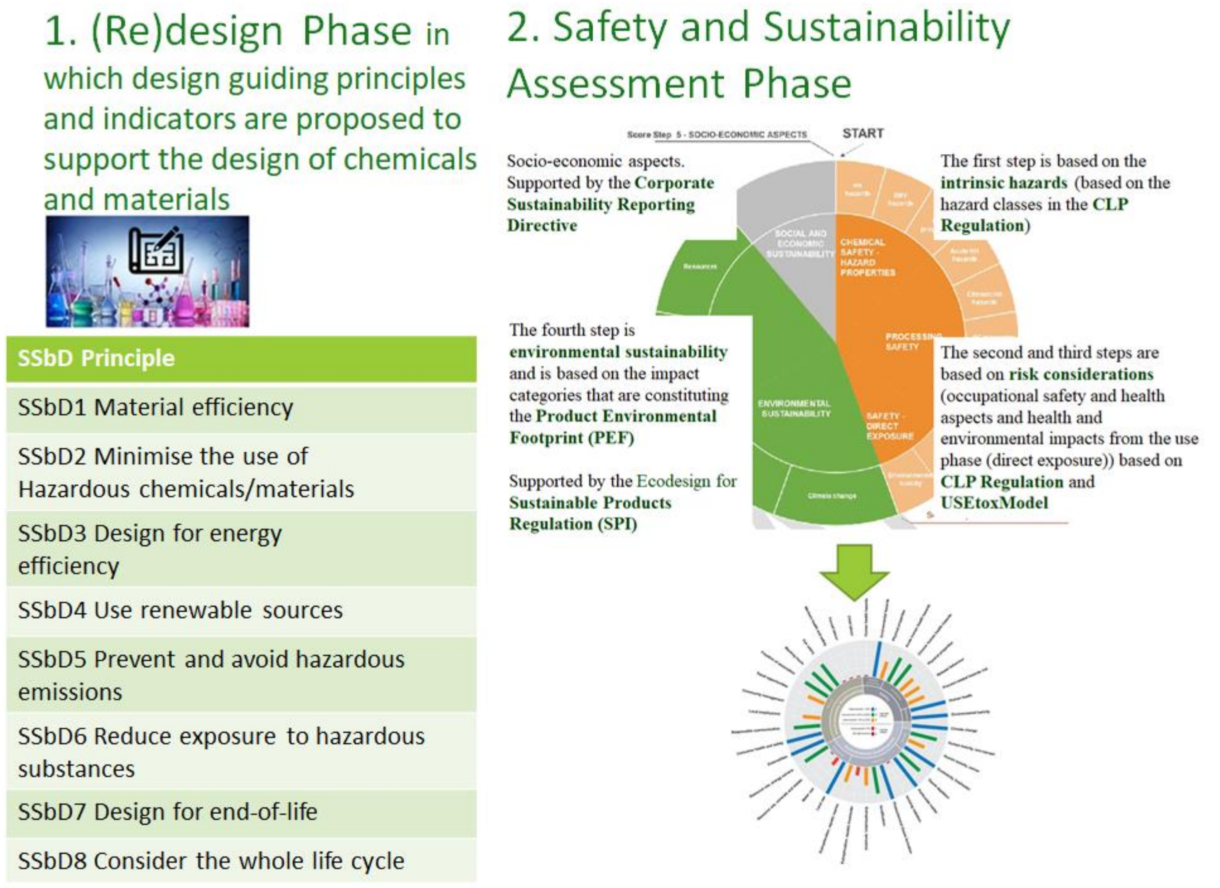

Figure 1. Two-phase process in the JRC framework for the definition of criteria and evaluation procedure for chemicals and materials (adapted from JRC Report, 2022 [1])

3.1 'by-design' phase

In the (re)design phase, SSbD principles have been identified by the EC JRC including:

1. *SSbD1 Material efficiency,*
2. *SSbD2 Minimise the use of hazardous chemicals/materials,*
3. *SSbD3 Design for energy efficiency,*
4. *SSbD4 Use renewable sources,*
5. *SSbD5 Prevent and avoid hazardous emissions,*
6. *SSbD6 Reduce exposure to hazardous substances*
7. *SSbD7 Design for end-of-life,*
8. *SSbD8 Consider the whole life cycle* [2].

Table 1 is a list of SSbD design principles and associated definition, and examples of actions and indicators that can be used in the design phase for the (re)design phase (Caldeira 2022).

Table 1. List of SSbD design principles and associated definition, and examples of actions and indicators that can be used in the design phase for the (re)design phase [1]

SSbD principle (based on)	Definition	Examples of Actions	Examples of indicators related to the SSbD principle (see Annex 2 for definition)
SSbD1 Material efficiency (GC2, CC2, GC8, GC9, GC5, CC5, GC1, SC2)	Pursuing the incorporation of all the chemicals/materials used in a process into the final product or full recovery inside the process, thereby reducing the use of raw materials and the generation of waste.	- Maximise yield during reaction to reduce chemical/material consumption - Improve recovery of unreacted chemicals/materials - Optimise solvent for purpose (amount, typology and recovery rate) - Select materials and processes that minimise the generation of waste - Minimise the number of chemicals used the production process - Minimize waste generation - Identify occurrence of use of Critical Raw Material[17], towards minimizing or substituting them	- Net mass of materials consumed (kg/kg) - Reaction Yield - Atom Economy - Material Intensity index - E-factor (%) -Purity of recovered solvent (%) - Solvent selectivity [-] - Yield of extraction (%) - Water consumption (m^3/kg) - Recycling efficiency/recovery rate (%) - Total amount of waste (kg/kg) - Amount of waste to landfill (kg/kg) - Critical Raw Material presence (yes/no)
SSbD2 Minimise the use of hazardous chemicals/materials (GC3, SC1, GR1, GC4, GE1, GR3, GC5)	Preserve functionality of products while reducing or completely avoid using hazardous chemicals/materials where possible.	- Reduce and/or eliminate hazardous chemicals/materials in manufacturing processes - Verify possibility of using hazardous chemicals/materials in close loops when they cannot be reduced or eliminated - Eliminate hazardous chemical/materials in final products	- Biodegradability of manufactured chemical/material - Classification of raw chemicals/materials as SVHC (yes/no)
SSbD3 Design for energy efficiency (GC6, CC4, GE4, GE5, CC8, GE8, GE10, GE3, GR7, GC8, GC9, CC10)	Minimise the overall energy used to produce a chemical/material in the manufacturing process and/or along the supply chain.	Select and / or develop (production) processes considering: - Alternative and lower energy intensive production/separation techniques - Optimize energy efficiency of solvent recovery - Maximise energy re-use (e.g. heat networks integration and cogeneration) - Fewer production steps (e.g applying lean thinking) - Use of catalysts, including enzymes - Reduce inefficiencies and exploit available residual energy in the process or select lower temperature reaction pathways	- Boiling temperature (°C) - Heat of vaporisation (MJ/kg) - Energy consumption (kWh/kg or MJ/kg) - Energy efficiency (%) - Solvent selectivity [-] - Yield of extraction (%)

SSbD principle (based on)	Definition	Examples of Actions	Examples of indicators related to the SSbD principle (see Annex 2 for definition)
SSbD8 Consider the whole life cycle (GE6, GR2, SC3, GR6, GR8)	Apply the other design principles thinking through the entire life cycle, from supply-chain of raw materials to the end-of-life in the final product	Consider for example: - Using reusable packaging for the chemical/material under assessment and for chemicals/materials in its supply-chain - Consider the most likely use of chemical/material and if there is the possibility to recycle it -. Energy-efficient logistics (i.e. reduction of transported quantities, change in mean of transport) - Reducing transport distances in the supply-chain -Applying responsible sourcing principles	- Recyclable? (yes/no) - Disassembly/reparability design (yes/no) - Durability (years) - Value-based resource efficiency indicator (VRE) - Material Circularity Indicator (MCI) - Biodegradability of manufactured chemical/material (yes/no)

GC: Green Chemistry Principle (Anastas and Warner, 1998), GE: Green Engineering Principles (Anastas and Warner,2003), SC: Sustainability Chemistry Criteria (UBA, 2009), GR: UBA Golden Rule (UBA, 2016), CC: Circularity Chemistry Principles (Keijer et al. 2019). See Annex 2 for information on the principles

In the context of the framework of SSbD criteria definition for chemicals and materials, the JRC report [1], defines the term 'by-design' in 3 levels:

1. <u>Molecular design</u>: this is the design of new chemicals and materials based on the atomic level description of the molecular system. This type of design effectively delivers new substances, whose properties may, in principle, be tuned to be safe(r) and (more) sustainable.
2. <u>Process design</u>: this is the design of new or improved processes to produce chemicals and materials. Process design does not change the intrinsic properties (e.g. hazard properties) of the chemical or material, but it can make the production of the substance safer and more sustainable (e.g. more energy or resource efficient production process, minimising the use of hazardous substances in the process). The process design includes upstream steps, such as the selection of the feedstock.
3. <u>Product design</u>: this is the design of the product in which the chemical/material might be used with a specific function that will eventually be used by industrial workers, professionals or consumers.

The development of a new chemical/material is often brought on through an innovation process that can be structured in stage-gate approach. **The process development can be monitored using the Technology Readiness Level (TRL) and at each stage quantitative and qualitative new information**

may be available for the assessment. The safety and sustainability assessment (green box, Figure 1 should be performed at early TRL (to the extent possible) to ensure that the application of the principles is indeed resulting in a good performance.

3.2 Sustainability assessment

Sustainability covers and integrates safety, economic, environmental, and social aspects to avoid harm to humans and the environment [3]. Sustainability also supports the EU Green Deal [4] whose ambitions include becoming climate neutral, protecting human life, animals and plants by cutting pollution, helping companies become world leaders in clean products and technologies and being inclusive helping ensure a just and inclusive transition [5]. '*In the context of chemicals, sustainability can be seen as the ability of a chemical, material, product or service to deliver its function without exceeding environmental and ecological boundaries along its entire life cycle, while providing welfare and socio-economic benefits* [2, 3]'.

In the sustainability assessment phase, five steps were provided for defining criteria for SSbD chemicals and materials. The first step is based on the intrinsic hazards (based on the hazard classes in the CLP Regulation). The second and third steps are based on risk considerations (occupational safety and health aspects and health and environmental impacts from the use phase (direct exposure)) based on CLP Regulation and USEtoxModel. The fourth step is environmental sustainability and is based on the impact categories that are constituting the Product Environmental Footprint (PEF) and it is supported by the Ecodesign for Sustainable Products Regulation (SPI) [6-8]. The fifth step would cover socio-economic aspects.

According to the JRC report [1], ***Environmental Sustainability*** refers to the ability to conserve natural resources and protect global ecosystems to support human health and well-being, within the limits of our Planet. Assessing environmental sustainability implies to assess the environmental impacts generated by chemicals/materials along the entire life cycle to move towards:

- **A toxic-free environment** as stated in the CSS (i.e. minimising the total toxicity footprint in terms of ecotoxicity and human toxicity - at each stage of the production and consumption life cycle, originated not only by the assessed chemical or material, but also by all the chemicals that are emitted along the life cycle);
- **A climate-neutral economy** (i.e. minimising the emission of greenhouse gases along the life cycle);
- **A resource efficient economy and a regenerative economy** (i.e. using natural resources in a sustainable manner, minimising inputs and waste generation, and providing more benefits than burdens);
- **The reduction of biodiversity loss and the conservation of ecosystem** functioning, addressing the main drivers of structural and functional biodiversity loss (e.g. land use, climate change).

Table 2 represents the components of the proposed SSbD criteria definition framework while

Table 3 shows a list of aspects and indicators (hazard properties) relevant for Step 1 in the Safety and Sustainability Assessment Phase (Caldeira 2022)). Finally, Table 4 shows the recommended models for the Environmental Footprint method including indicator, units and models (adapted from (Caldeira 2022)). This last point is developed in SURPASS deliverable D4.5 on "Methodology and results for LCA and LCC – Initial".

Table 2. Components of the proposed SSbD criteria definition framework (adapted from JRC Report, 2022 [1])

Step	Assessment Dimension	Assessment aspects	System Scope	Aspect/Indicator	Criteria
1	**Hazard assessment**	The assessment focuses on the hazard properties (human health, environmental and physical hazards) of the manufactured chemicals and materials	Chemical/Material intrinsic properties	See Table 3	See Section 4.4.1 and Table 4
2	**Human health and safety aspects in the production and processing phase**	Assessment of the human health and safety aspects during the production phase of the chemical/material from the used raw materials (production) and the manufactured chemical/material (processing, waste stage).	Chemical/material production and processing	See Section 4.2.2	See Section 4.2.2
3	**Human health and environmental aspects in the final application phase**	This step evaluates the human health and environmental impacts during the chemical/material final application phase.	Chemical/material application	See section 4.2.3	The indicator values should be below the safe levels. For details see section 4.2.3.
4	**Environmental sustainability (Life Cycle Assessment)**	Assess life cycle environmental impact categories for: Toxicity and Eco-toxicity Climate Change Ozone Depletion, Particulate Matter, Ionising radiation, Photochemical Ozone Formation, Acidification, Eutrophication Resources, Land Use, Water Use	Chemical/Material entire life cycle	See Table 7	Reduction by X% compared to the current state of the art for intended use. The 'X' might differ depending on the impact category. For details see section 4.2.4.
5	**Social Sustainability, Economic Sustainability**	This step is at an exploratory phase. It present an overview of social aspects that could be considered in the future. For the economic pillar, the step focuses on non-financial aspects, i.e. the identification and monetization of externalities arising during the life cycle of a chemical or a material.	Chemical/Material entire life cycle (for the economic part) Chemical/Material production and relevant suppliers (for the social part)	See Table 10 for examples	To de defined.

Table 3. List of aspects and indicators (hazard properties) relevant for Step 1 in the Safety and Sustainability Assessment Phase [1])

Group definition	Human health hazards	Environmental hazards	Physical hazards
Includes the most harmful substances (according to CSS (EC, 2020a)), including the substances of very high concern (SVHC) according to REACH Art. 57(a-f)[20],[21] (EU, 2006). These hazard properties form Criterion H1.	• Carcinogenicity Cat. 1A and 1B • Germ cell mutagenicity Cat. 1A and 1B • Reproductive / developmental toxicity Cat. 1A and 1B • Endocrine disruption Cat. 1 (human health) • Respiratory sensitisation Cat 1 • Specific target organ toxicity - repeated exposure (STOT-RE) Cat. 1, including immunotoxicity and neurotoxicity	• 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 (environment)	
Includes substances of concern, as described in CSS (EC, 2020a), defined in the Article 2(28) of SPI proposal (EC, 2022b)[22] and that are not already included in Criterion H1. These hazard properties form Criterion H2.	• Skin sensitisation Cat 1 • Carcinogenicity Cat. 2 • Germ cell mutagenicity Cat. 2 • Reproductive / developmental toxicity Cat. 2 • Specific target organ toxicity - repeated exposure (STOT-RE) Cat. 2 • Specific target organ toxicity - single exposure (STOT-SE) Cat. 1 and 2 • Endocrine disruption Cat. 2 (human health)	• Hazardous for the ozone layer • Chronic environmental toxicity (chronic aquatic toxicity) • Endocrine disruption Cat. 2 (environment)	
Includes the other hazard classes not part already in Criteria H1 and H2. These hazard properties form Criterion H3.	• Acute toxicity • Skin corrosion • Skin irritation • Serious eye damage/eye irritation • Aspiration hazard (Cat. 1) • Specific target organ toxicity - single exposure (STOT-SE) Cat. 3	• Acute environmental toxicity (acute aquatic toxicity)	• Explosives • Flammable gases, liquids and solids • Aerosols • Oxidising gases, liquids, solids • Gases under pressure • Self-reactive • Pyrophoric liquids, solid • Self-heating • In contact with water emits flammable gas • Organic peroxides • Corrosivity • Desensitised explosives

Criteria	Description	Observations (in alignment with CSS)
Criterion H1	The criterion refers to the **most harmful substances**, according to CSS, including the substances of very high concern (SVHC) according to REACH Art. 57(a-f) and additional hazard properties, as defined in Table 3. This is a cut-off criterion, establishing a minimum set of hazard requirements that need to be fulfilled by a chemical or material in order to be considered eventually SSbD after the other assessments are performed. Therefore, the assessment of the other aspects can be performed in order to understand the overall SSbD performance (e.g. safety during the use assessed in Step 3, other environmental sustainability aspects assessed in Step 4) if this helps the innovation process.	The chemicals and materials which do not pass this criterion should be: - Prioritised for substitution - Re-designed in order to reduce their adverse effects - Only allowed in uses proven essential for society (e.g. if their use is necessary for health, safety or is critical for the functioning of society and if there are no alternatives that are acceptable from the standpoint of environment and health)[24] - Safely used and emissions/exposure be controlled along the whole life cycle while activities are undertaken to develop alternatives as soon as possible and their use is phased out as soon as less hazardous alternatives are available - Tracked through their life cycle
Criterion H2	The criterion refers to the hazard class categories and hazardous substances which are part of the **substances of concern** described in CSS and not included already in criterion H1, as defined in Table 3. For the chemicals or materials with hazard properties a safety level or score will be assigned, while the SSbD assessment will continue with the evaluation of the other safety and sustainability aspects, in order to assess their overall SSbD performance.	The chemicals and materials that do not pass this criterion should be: - Substituted as far as possible - Re-designed in order to reduce their adverse effects - Safely used and emissions/exposure be controlled along the whole life cycle, until less hazardous alternatives are available - Tracked through their life cycle
Criterion H3	The criterion refers to the group of **other hazard classes**, including here all hazard properties not covered by criteria H1 and H2, as defined in Table 3. Following a similar approach described above, a safety level or score will be assigned to the chemicals or materials under this category in order to be integrated in the overall SSbD assessment.	The chemicals and materials that do not pass this criterion should be: - Flagged for review and eventually reduce toxic effects - Ensure their safety along the life cycle until less hazardous alternatives are available

Table 4. Recommended models for the Environmental Footprint method including indicator, units and models (adapted from [1])

LCA Assessment level	Impact category	Indicator	Unit	Recommended default LCIA model
Toxicity	**Human toxicity, cancer effects**	Comparative Toxic Unit for humans (CTU_h)	CTUh	based on USEtox2.1 model (Fantke et al., 2017) adapted as in (Saouter et al., 2018)
	Human toxicity, non-cancer effects	Comparative Toxic Unit for humans (CTU_h)	CTUh	based on USEtox2.1 model (Fantke et al. 2017), adapted as in Saouter et al., 2018)
	Ecotoxicity freshwater	Comparative Toxic Unit for ecosystems (CTU_e)	CTUe	based on USEtox2.1 model (Fantke et al. 2017), adapted as in Saouter et al., 2018)
Climate Change	**Climate change**	Global warming potential (GWP100)	kg CO_2 eq	Bern model - Global warming potentials (GWP) over a 100-year time horizon (based on (IPCC, 2013)
Pollution	**Ozone depletion**	Ozone Depletion Potential (ODP)	kg CFC-11eq	EDIP model based on the ODPs of the World Meteorological Organisation (WMO) over an infinite time horizon ((WMO, 2014)+ integrations)
	Particulate matter/Respiratory inorganics	Human health effects associated with exposure to $PM_{2.5}$	Disease incidences[37]	PM model (Fantke et al., 2016) in (UNEP, 2016)
	Ionising radiation, human health	Human exposure to ^{235}U	kBq ^{235}U	Human health effect model as developed by Dreicer et al., 1995 (Frischknecht et al, 2000)
	Photochemical ozone formation	Tropospheric ozone concentration increase	kg NMVOC eq	LOTOS-EUROS (Van Zelm et al., 2008) as applied in ReCiPe 2008
	Acidification	Accumulated Exceedance (AE)	mol H+ eq	Accumulated Exceedance (Posch et al., 2008; Seppälä, et al., 2006)
	Eutrophication, terrestrial	Accumulated Exceedance (AE)	mol N eq	Accumulated Exceedance (Seppälä et al. 2006, Posch et al, 2008)
	Eutrophication, aquatic freshwater	Fraction of nutrients reaching freshwater end compartment (P)	kg P eq	EUTREND model (Struijs, et al. 2009)as implemented in ReCiPe 2008
	Eutrophication, aquatic marine	Fraction of nutrients reaching marine end compartment (N)	kg N eq	EUTREND model (Struijs et al, 2009) as implemented in ReCiPe 2008
Resources	**Land use**	Soil quality index[38] aggregating: Biotic production, Erosion resistance, Mechanical filtration and Groundwater replenishment	Dimensionless*	Soil quality index based on LANCA model (De Laurentiis et al., 2019) and on the LANCA CF version 2.5 (Horn and Maier, 2018)
	Water use	User deprivation potential (deprivation weighted water consumption)	m^3 water eq of deprived water	Available WAter REmaining (AWARE) model (Boulay et al., 2018; UNEP, 2016)
	Resource use, minerals and metals	Abiotic resource depletion (ADP ultimate reserves)	kg Sb eq	CML (Guinée et al., 2002) and (Van Oers et al. 2002)
	Resource use, energy carriers	Abiotic resource depletion – fossil fuels (ADP-fossil)[39]	MJ	CML (Guinée et al., 2002) and (Van Oers et al. 2002)

*dimensionless index[40] resulting from the aggregation of the individual indicators for soil covering: biotic production (kg biotic production/ (m^2*a)); Erosion resistance (kg soil/ (m^2*a)); mechanical filtration (m^3 water/ (m^2*a)); and groundwater replenishment (m^3 groundwater/ (m^2*a)).

According to the JRC report [1], ***Social Sustainability*** is well reflected in the SDGs framework which comprises a globally agreed list of objectives and targets to be pursued for achieving sustainable development. In the SDGs framework, several Goals focus on social aspects, e.g. poverty eradication (SDG 1), food security (SDG 2), health (SDG 3), education (SDG 4), gender equality (SDG 5), decent work (SDG 8), reduce inequalities (SDG 10), peace and justice (SDG 16). Other SDGs, while referring to environmental or technological aspects, have a clear link with social aspects, like those related to water and sanitation (SDG 6) and access to energy (SDG 7).

According to the JRC report [1], ***Economic Sustainability*** refers to multiple aspects related to techno-economic feasibility, to operational costs, etc. Moreover, there are important considerations to be made in the context of SSbD such as the 'availability' of raw materials, as chemicals/materials cannot be declared SSbD if the raw materials to produce them are not renewable or are (very) scarce and extracted and processed in an unsustainable manner. Economic aspects play a role when there is a need to rank chemicals and materials based on SSbD criteria (even if they are not SSbD). However, mainly externalities consideration[2] is at stake in a sustainability framework like the SSbD one.

3.3 A new understanding of safety

The safety concept is related to the absence of unacceptable risk for humans and the environment by avoiding the use of hazardous chemicals [2]. In the EU-CSS, the ambitions towards a toxic-free environment and protection against the most harmful chemicals are evident. An important development is the extension of the generic approach to risk management to ensure that chemicals that cause cancers, gene mutations, affect the reproductive or the endocrine system, or are persistent and bioaccumulative, are not present in consumer products. This generic approach will be extended to other harmful chemicals including those affecting the immune, neurological or respiratory systems and chemicals toxic to specific organs [9]. The scope of this EU-CSS is also to protect vulnerable groups which typically include pregnant and nursing women, the unborn, infants and children, the elderly people as well as workers and residents subject to high and/or long term chemical exposure [9].

[2] Consumption, production, and investment decisions of individuals, households, and firms often affect people not directly involved in the transactions.

4 Development of the SURPASS SSRbD strategy and methodology for polymeric materials

In this section, a description of the SURPASS safe, sustainable, and recyclable by design (SSRbD) strategy and methodology is provided. It was developed through several co-creation sessions with the SURPASS consortia and organized by T4.1 members. An important consideration is that SURPASS is developing and implementing this strategy at the same time, and here a first draft description is provided which will be adapted as we apply it to the SURPASS case studies. Figure 2 shows the general life cycle thinking approach used in developing the SURPASS SSRbD strategy which integrates innovation/functionality with safety and sustainability in an iterative process.

Figure 2 General life cycle thinking approach taking into account the innovation process and integrating innovation (functionality) with safety and sustainability in an iterative process.

4.1 Applying the SSbD Framework to SURPASS Project

The translation of the EC JRC framework to fit SURPASS Project was performed through the development of a holistic life cycle thinking. The Safe-Sustainable-and-Recyclable-by-Design Approach consists of the following steps (Figure 3):

1. The identification of criticality, toxicity, environmental, social, circularity, functionality and economic impacts in a life cycle thinking perspective per case study
2. The development of Safe-Sustainable-and-Recyclable-by-Design strategies
3. Verification of Safe-Sustainable-and-Recyclable-by-Design strategies to ensure they lead to safer and more sustainable alternatives

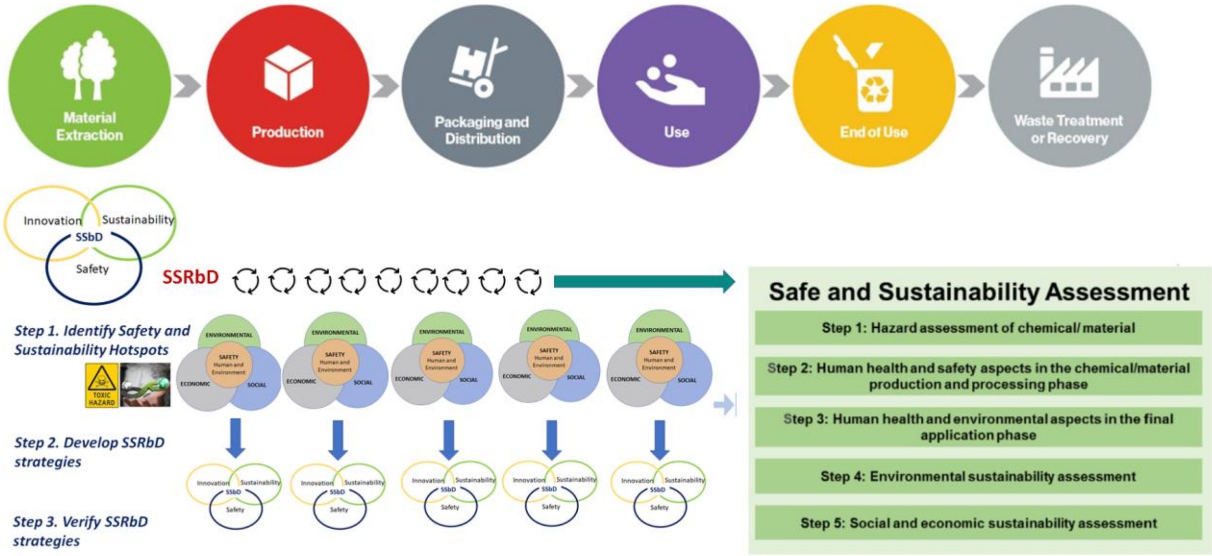

Figure 3. SURPASS approach for the translation of the JRC framework for SSbD criteria to practical operationalization

The SSRbD methodology in Figure 3 will be applied to the three case studies of the SURPASS Project, and has been adapted to each application and domain. It is important to note that this report shows 3 steps, where Steps 1 and 2 of the methodology (the 'design-phase in the JRC Framework). Step 3 (analogous to the Safety and Sustainability Assessment in the JRC framework, steps 1-5) will be performed throughout the project.

4.2 The 'big picture', Step 1, Identification of value chain safety & sustainability challenges

This first step consists of the identification of criticality, toxicity, environmental, social, circularity, functionality and economic impacts in a life cycle thinking perspective per case study. For each of the case studies, the biggest safety & sustainability challenges were identified.

- → ***Building sector, Case Study CS#1:*** New recyclable-by-design bio-sourced polyurethane (PU) to replace PVC (Polyvinyl Chloride) as insulating material for window frames (Table 5).
- → ***Transport sector, Case Study CS#2:*** Fire resistant, intrinsically recyclable epoxy-vitrimer materials for sustainable composites to replace metal for train body (Table 6).

Packaging sector, Case Study CS#3: Recyclable MultiNanoLayered (MNL) films to replace multi-layer films for packaging with drastically reduced concentrations of compatibilizers (

→ Table 7).

Table 5. Baseline Generation: Identification of safety and sustainability issues/hotspot for the Building sector Case Study

	Life cycle stage			
	Raw material and resources	**Processing and manufacturing**	**Use**	**End-of-life**
Environmental impact	Polyamines are toxic for aquatic organisms and accidental release need to be considered. Impregnation solvents (can be alcohols) during the vitirmerization process that have an impact as VOC + are flammable and ocular irritants Integration of catalysts (IAS) in the polymer can increase the production of NIAS + release catalyst In 23rd of August 2023 there will be training needed for the use of diisocyanates https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:32020R1149	Solid polyurethane residues (powder, chips) during window assembly Compression moulding is done at high temperatures and actual situation needs to be considered Use of recycled input, recycling process more complex than existing manufacturing process will need more qualified workers, manipulation of chemicals (even non-toxic) can lead to a disapproval of the process	Rigid polyurethane foams will, when ignited, burn rapidly and produce intense heat, dense smoke and gases which are irritating, flammable and/or toxic. Polyurethanes form carbon monoxide, hydrogen cyanide and other toxic products on decomposition and combustion. Solid polyurethane residues (chips) during window assembly	
Social impact	Bio-based components (bio-polyols needed in INDRESMAT formulation): potential land use competition (feedstock)	Isocyanate extension and synthesis of poly(oxime-urethane) require more steps and more high-quality job positions.		
Health-safety impact	Catalysts are organic or acid bases, they are classified as corrosive and can be irritant for lungs when used as powders. Isocyanate, which is a main component in PU synthesis, needs to be used by specially trained employees due to its effect on human health https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:32020R1149 A prominent example of PU vitrimer chemistry uses toxic catalysts, for example dibutyltin dilaurate, a tin-based catalyst	window assembly tools can be dangerous to handle, sanding of the window frames could release fine dust particles which can harm the respiratory tract, solvent based paints (for windows) compression molding: considerations due to the high temperatures used (burning) and potential toxic vapours generation grinding (fine powders possibly affect the airway), impregnation (chemicals, solvent, temperature for drying solvents), extrusion (mechanical hazard, high temperature (160-200°C))	Isocyanates are toxic and it compulsory that <1ppm of isocyanate group are unreacted in the final product. Integration of catalysts (IAS) in the polymer can increase the production of NIAS + release catalyst	
Economic impact	Bio-based components are not produced at large scale as much as fossil-based materials, therefore they could be more expensive Fossil-based components depend directly on rising transport cost which is related to rising energy price due to Russia-Ukraine war Poly(oxime-urethane) strategy requires more expensive materials than traditional PU and PVC	Energy consumption is expected to be higher than with the use of usual manufacturing process (grinding, impregnation and extrusion/foaming vs molding/foaming), a compromise between energy consumption and toxicity/flammability of solvents will be done for impregnation step	Polyurethane products require larger investment from the end user than commodities: raw materials price volatility due to oligopoly nature of polyurethane market	

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SURPASS

Table 6. Baseline Generation: Identification of safety and sustainability issues/hotspot-Transport sector Case Study

Baseline Generation: Identification of safety and sustainability issues/hotspot	**Life cycle stage**			
	Raw material and resources	**Processing and manufacturing**	**Use (product)**	**End-of-life (product)**
Environmental impact	**The epoxy resin** (derived from the condensation reaction between epichlorohydrin and bisphenol-A) is fossil feedstock (from petroleum). At uncured stage, can give off fumes when it is applied or heated, and can also leach chemicals into the ground and water. **Di-amine hardener** is made from petroleum products. No environmental impact identified for the time being (it is not classified in REACH). The synthesis process of both, leaves a large CO_2 footprint.	**Epoxy resin**, at uncured stage, can give off fumes when it is applied or heated, and can also leach chemicals into the ground and water, contributing to land and water polution	**The composite manufacturing** by Prepreg process : medium-low throughput process	epoxy-based composites at the end of their life are burned or stored in landfills. The burning of these materials contributes to significant energy consumption as well as releasing harmful gases such as CO2, further accentuating the greenhouse effect. On the other hand, the storage of these materials in landfills occupies and pollutes natural areas.
Health-safety impact		**Epoxy resins** give off fumes when it is applied or heated. These fumes can be harmful to the people who work with epoxy resin.	**Cured Epoxy resin:** The epoxy resin once reacted with the curing agent, the final product is not harmful as it does not off-gas during its life cycle.	
	Halogen fire retardant additives (toxic)	**Use of Halogen additives** during processing manufacturing and life-cycle: hazardous health impact of halogenated compounds, particularly on the endocrine system of people exposed to this product (workers and civilians).		
Social impact				
Economic impact	these flame retardant additives are based on fossil raw materials, which are exhaustible, and many of them are not present in Europe.			Major investment in incineration and landfill plants for disposal/minimisation of waste material
	Flame retardants and hardener are not produced at large scale, therefore they could be more expensive and insufficient			

Table 7. Baseline Generation: Identification of safety and sustainability issues/hotspot-Packaging sector Case Study

	Life cycle stage			
	Raw material and resources	**Processing and manufacturing**	**Use**	**End-of-life**
Environmental impact	Climate Change: Emission of Greenhouse Gases Fossil feedstock Water use environmental indicator (PEF)	Energy use - fossil fuels (MJ) Water use environmental indicator (PEF) Waste generation (kg/kg) Release of monomers and Volatile Organic Compounds (VOC)	Single Use product Consumer awareness on environmental impacts	Complex Waste Collection and sorting system Recycling efficiency/recovery rate (%) Amount of waste to landfill (kg/kg) Critical extract from decontamination processes
Social impact	Child labour	Assessment of accident at work	Awareness about the overconsumption Pollution in third world countries (export of critical residues)	
Health-safety impact	Absence of most harmful substances according to CSS (EC, 2020) and SVHC of REACH Art. 57 (EU, 2006)	Risk assessment at the workplace	Likehood of human exposure and potential route (inhalation, dermal, ingestion) Environmental hazard: Specific Environmental Release Categories (SpERCs)	Potential presence of contaminants or hazardous substances in product waste Existing recycling and treatment of contaminated packaging
Economic impact	Economic crisis impact on fossil prices	Economic crisis impact on fossil prices-> Higher raw material's prices-> Higher final product prices		Value of recycled materials vs. undesired effects limiting the value of the PE waste stream

4.3 Development of possible SSRbD strategies (Step 2)

This chapter focuses on the development of 'by-design' strategies (analogous to the (re)design phase of the JRC framework. Here we discuss important characterisation parameters for polymeric materials, functionality challenges and development of SSRbD strategies leading to the development of a global practical approach to support the development of SSRbD strategies. For each case study, we show how in SURPASS, we try to balance between functionality with safety and sustainability in an iterative way to obtain safe and sustainable by design strategies. We also show the mapping of the SSbD Approach applied to each Case of Study of SURPASS Project.

4.3.1 Characterisation of polymeric materials

The characterisation of polymeric materials should include:

- Polymer class: classification of polymers based on properties (e.g. thermoplastics or thermosets).
- Polymer type: a specific sort of polymer within a polymer class (e.g. PET or PP).
- Grade and purity: a specific structure and molecular mass within a polymer type and purity.
- Additives: substances added to the polymer to improve its properties (e.g. pigment or flame retardant).
- Blends: combination of polymers (e.g. thermoplastic-thermoplastic blend).
- Production residues: substances that do not deliberately remain in the material (e.g. catalyst or monomer).
- Non-intentionally added substances (NIAS): substances that have not been deliberately added to the material or unplanned new substances resulting from contact to other materials (e.g. due to degradation substances that leach into the material).

An inventory of substances analysed in SURPASS will be made including characterization data.

4.3.2 Functionality challenges and development of SSRbD strategies

4.3.2.1 Development of a global practical approach to support the development of SSRbD strategies

SSRbD has to be conducted in parallel to the eco-ideation and eco-selection steps for the innovative developments of plastics. The solution adopted and presented here corresponds to the implementation of the JRC SSbD framework for chemicals and materials in a global practical approach, which takes into account the development of complex systems in industry. Thus, a global SURPASS approach was developed to link product or material functionality with the innovation process for the development of SSRbD strategies. This is an iterative approach for balancing functionality with safety

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and sustainability aspects.

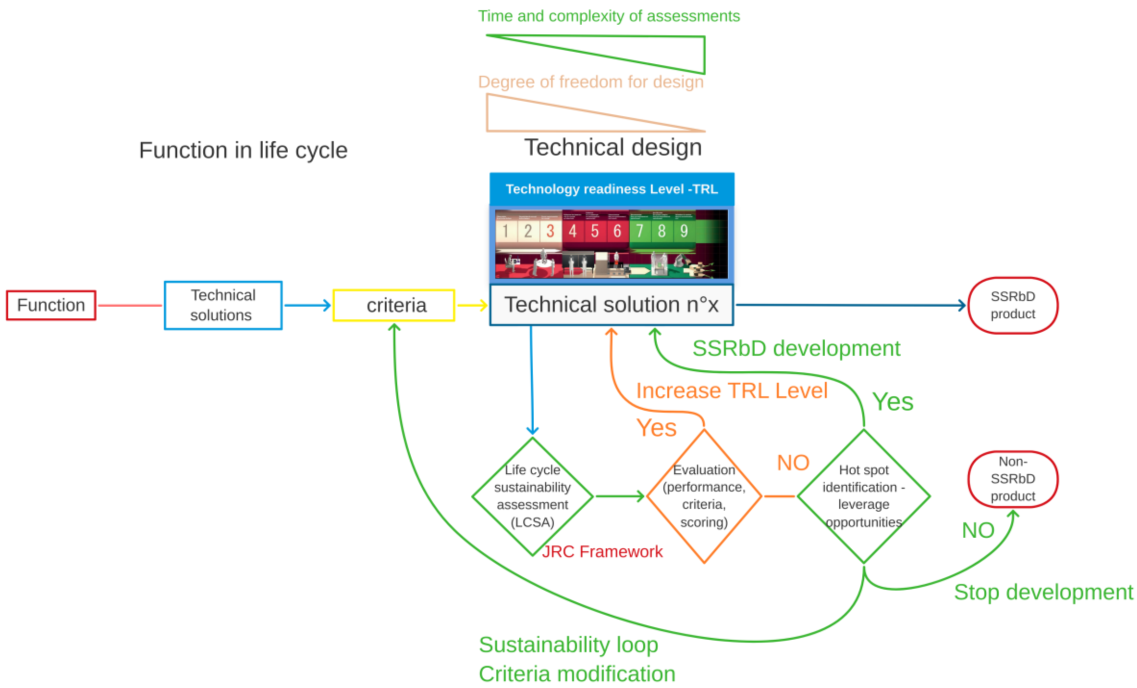

Figure 4 is a simplified diagram of the approach that highlights the decision tree to drive the sustainable assessments along the innovation process.

The construction of this approach uses elements from CEN 1325 [10], ISO 15686-5 and JRC framework to be easily integrated into companies environmental management systems. The full approach is presented Figure 5 and it will be explained in detail step by step in Figure 6 to Figure 10.

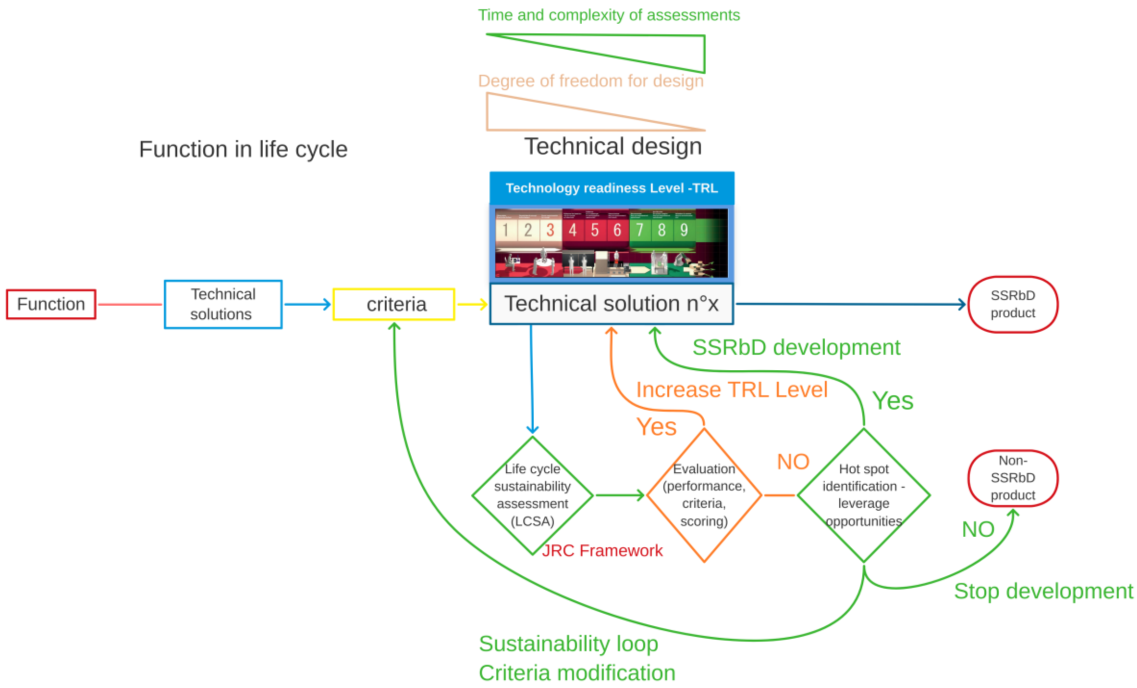

Figure 4. Simplified global SURPASS SSRbD practical approach

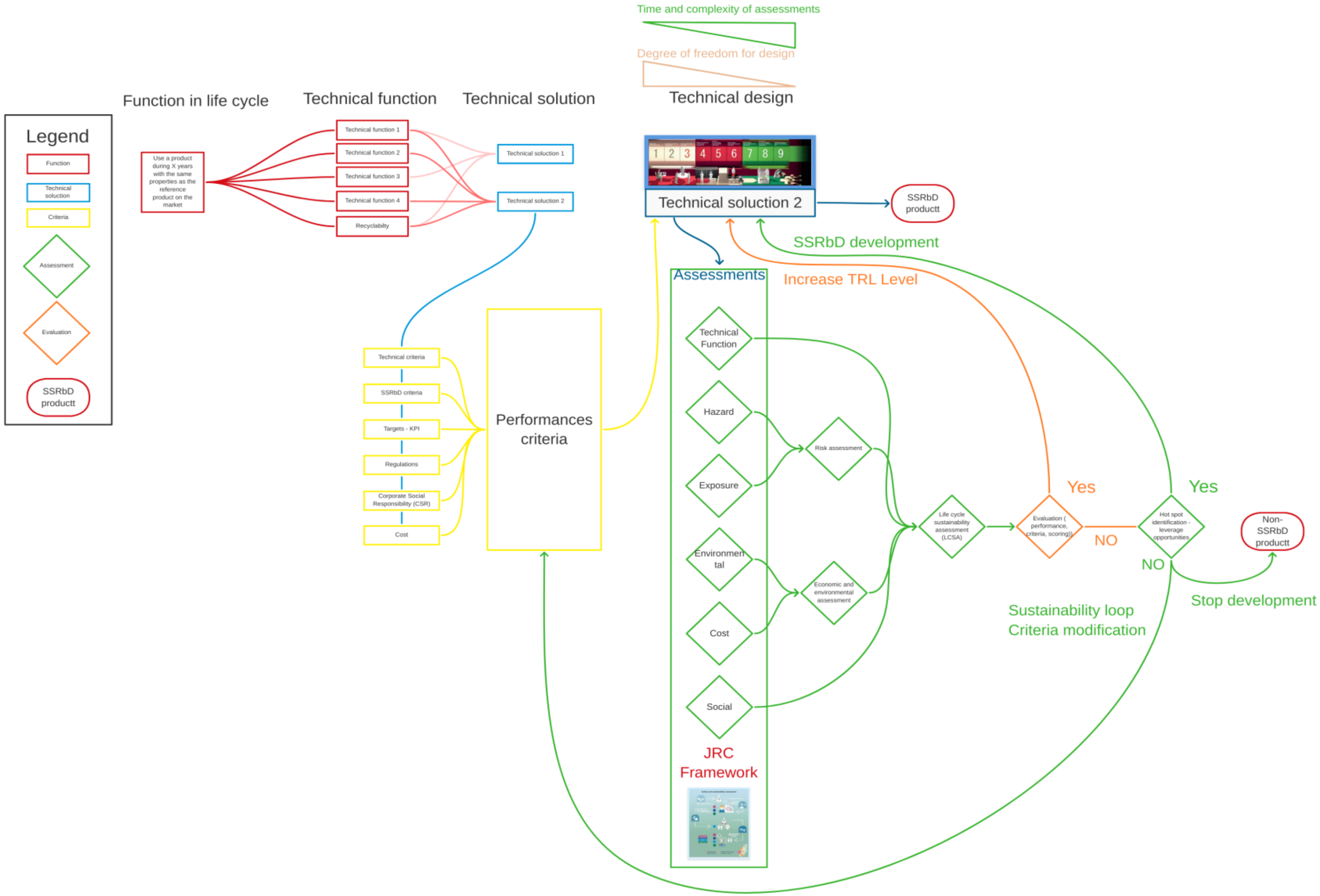

Figure 5. Detailed global SURPASS SSRbD practical approach

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The first step in the global approach is shown in Figure 6. It consists in performing a functional analysis of the product to define the function in a life cycle perspective (functional unit), then listing technical function requirements for the function and listing the technical solutions that fulfil the technical functions. It is noteworthy that a recyclability technical function is always included in these approach (Figure 6).

As an example taken from SURPASS CS#1, the life cycle function could be to use an SSRbD window for 10 years with the same properties as a PVC window. The technical functions associated are then thermal insulation, acoustic insulation, physical protection and recyclability. The technical solutions that correspond to these technical functions are a glass panel and a plastic frame.

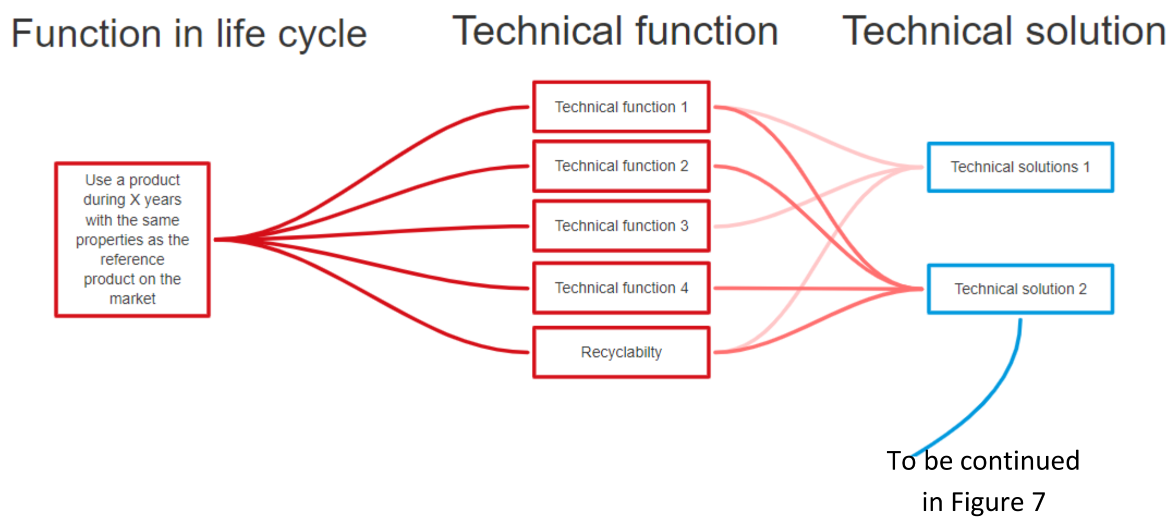

Figure 6. Functional unit and technical solution

The second step is shown on Figure 7. It defines performance criteria for the technical solutions. The main criteria, although not exhaustive, are related to technical, SSRbD, KPI, regulations, corporate social responsibility or cost.

For the window example, some criteria for the plastic frames are:

- *Technical criteria: a thermal transmittance of frames/profiles (EN ISO 10077-2:2017) equal to 0,81 W/(m^{2}K) (a Class 3 for air permeability)*
- *SSRbD criteria: an increase in durability of 35-45 years (20-30% increase compared to PVC), ≥ 40% thanks to bio based and renewable raw materials use*
- *Cost criteria: calculated cost of material less than 20% higher than PVC*

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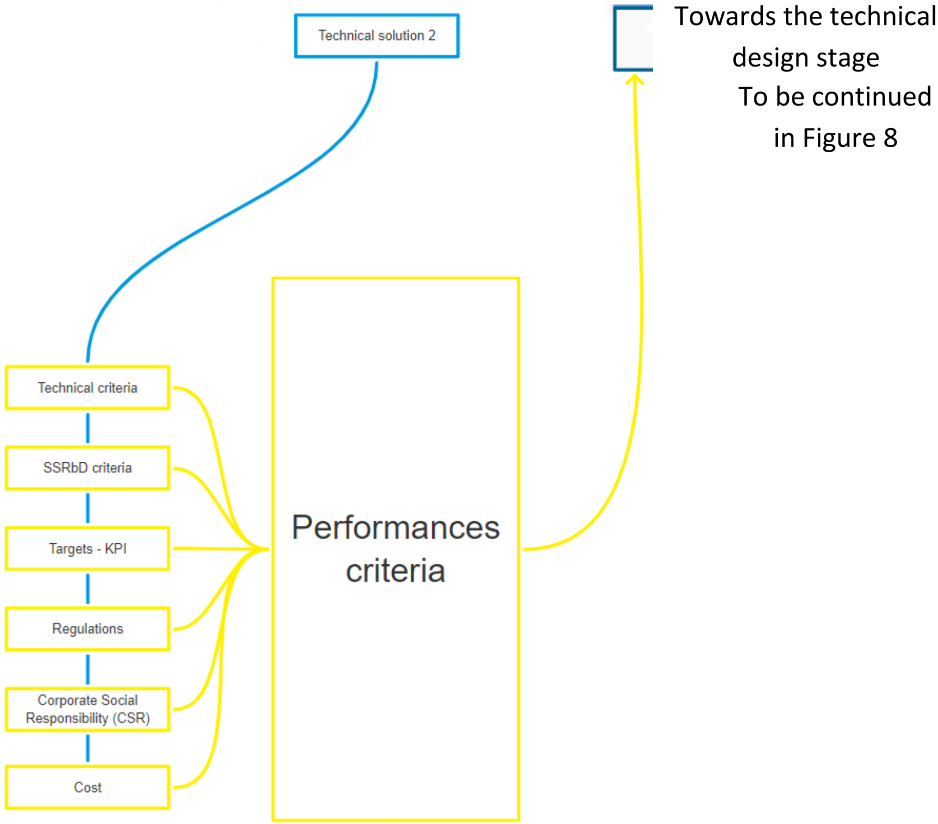


Figure 7. Criteria

The next part is the core of the SURPASS global practical approach with the Technical Design phase as can be seen on Figure 8. The Technical Design phase is strongly linked to the Technology Readiness Level (TRL) of the Technical solution. The technology maturity level (TRL) is a method of understanding the technical maturity of a technology during its development. The TRL level provides a coherent reference that can be understood by everyone, regardless of their skills. The upper part of the figure, above the TRL scale, shows that the lower the TRL of a technical solution, the greater the degree of freedom in technical developments and the less complex the sustainability assessments with a low level of information required. Conversely, the higher the TRL of a technical solution, the lower the degree of freedom in developments and the more complex the sustainability assessments but with a high level of available information. In the SURPASS project, the TRL levels of the CSs range from 3 to 5. In order to operationalise the assessment, a tiered approach with the realisation of three assessment loops was chosen. The loops are “early in the innovation process”, “mid in the innovation process” and “late in the innovation process”.

Thus, the performance criteria (yellow arrow) are introduced for technical solution 2 and the blue arrow moves towards the evaluation stage. As the technical design is at the core of the SSRbD iterative process, two more arrows could enter the technical design stage: the orange one when evaluation is successful to meet the expected performances and allows an increase in TRL level, and the green arrow when further SSRbD developments are needed to pass the evaluation. Finally, a second blue arrow points to the SSRbD product when life cycle sustainability assessment passes through the technical design loops and reaches the final TRL level.

For the window example, the criteria described above are introduced in the technical design stage to develop a new vitrimer for the window frame. If the assessment is successful (Orange arrow,) the TRL *level of the designed product increases towards the final product. This means that the solution meets targets in terms of transmission, permeability, durability and percentage of content for renewable and bio-based raw materials. If the assessment is not fully successful (for example if the recyclability level does not reach the target), further SSRbD developments are required and a new assessment has to be conducted.*

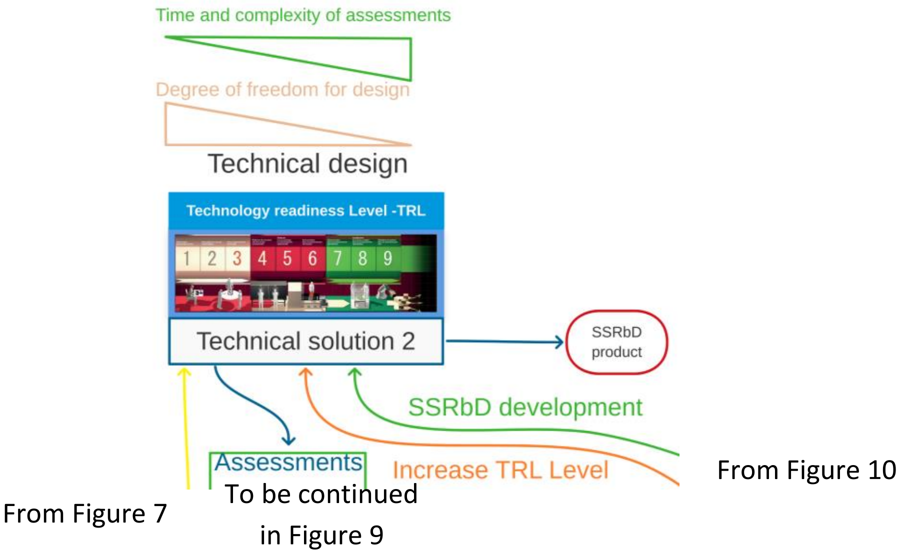


Figure 8. Technical design

The Figure 9 shows the assessment step following by the JRC framework. The choice made in the SURPASS project is to perform parallel assessments, an option indicated by JRC in the presentation of the Framework, rather than sequentially. This choice is based on the consortium knowledge on safe by design activities conducted in several projects (Serenade, SBD4, SAbyNA, [11, 12]). During the innovation process, evaluations should be as agile and quick as possible to identify hotspots and gaps to propose corrective solutions.
Hazard and Exposure are merged to give the Risk assessment and cost and environmental assessments are merged to give the Economic and environmental assessment. Then all assessments allow the Life cycle sustainability assessment (LCSA).

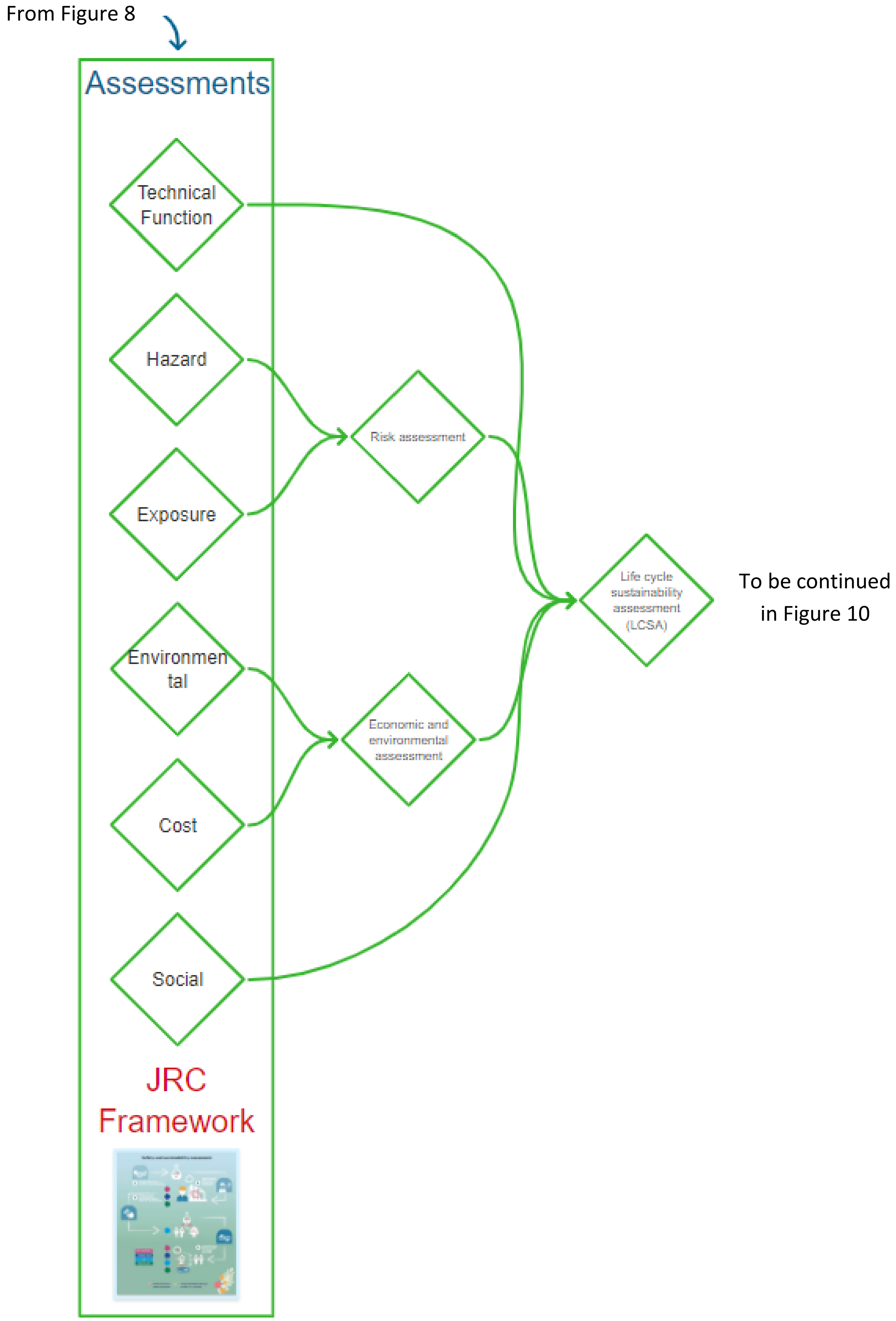


Figure 9. Assessments towards LCSA

The life cycle sustainability assessment is afterwards evaluated against the criteria defined for the product design as can be seen in Figure 10. If the life cycle sustainability assessment is successful, the

TRL of product design increases. If not, there is a step for hotspots identification and definition of leverage opportunities. If the identification is successful, further SSRbD developments are implemented and a new assessment loop is performed. Otherwise, there are two options, the first being to reassess and adapt the performance criteria and then perform a new assessment loop, and the second being to stop the product development.

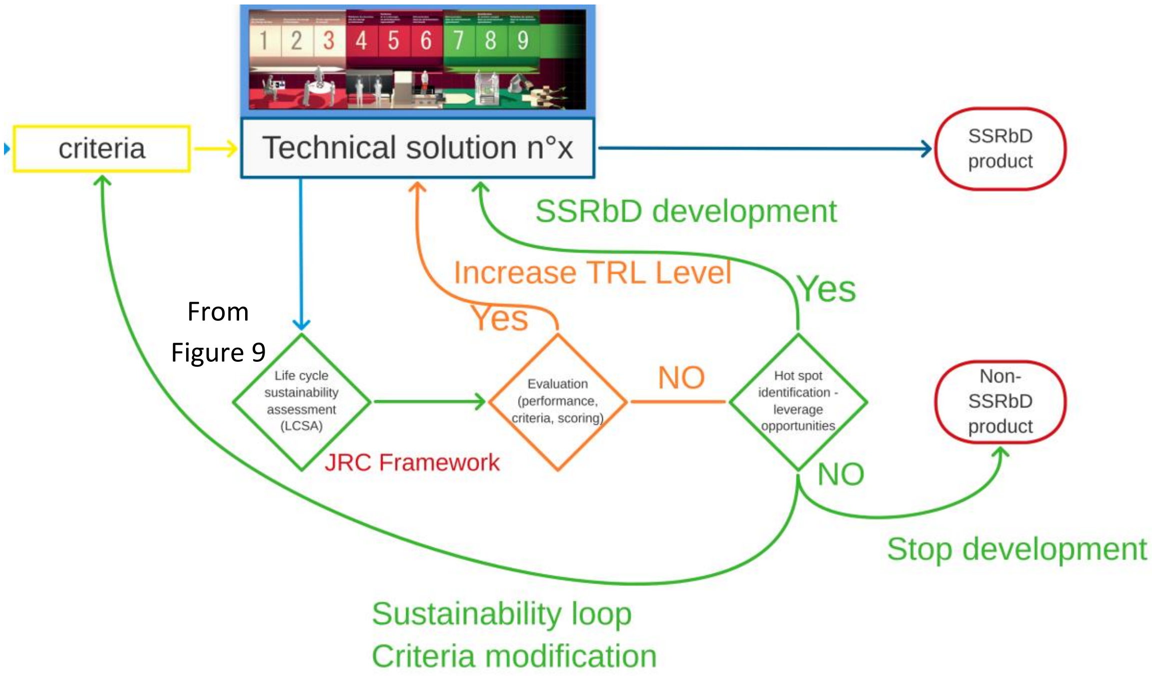


Figure 10. Evaluation

This SURPASS Global SSRbD practical approach allows to integrate SSRbD assessment in the innovation process for the development of a material from an early stage of the development. Thus, conduct assessments in parallel allows to have a tier approach and realised assessment at different levels of complexity as a function the development stages of the product or the criteria to be achieved.

The next step of operationalisation is presented in the following paragraphs of this report and in deliverable D4.5 on LCA and LCC methodology and results, applicable to the SURPASS case studies (initial version). It consists in establishing life cycle and development diagrams of the technical solutions. These diagrams will also be used to collect the Life Cycle Inventories (LCI).

For a description of process diagram of SURPASS CSs and template of Life Cycle and Development Diagram (LCDD) you can refer to Deliverable D4.5.

4.3.2.2 CS#1 Construction (Bio-based PU to replace PVC window frames)

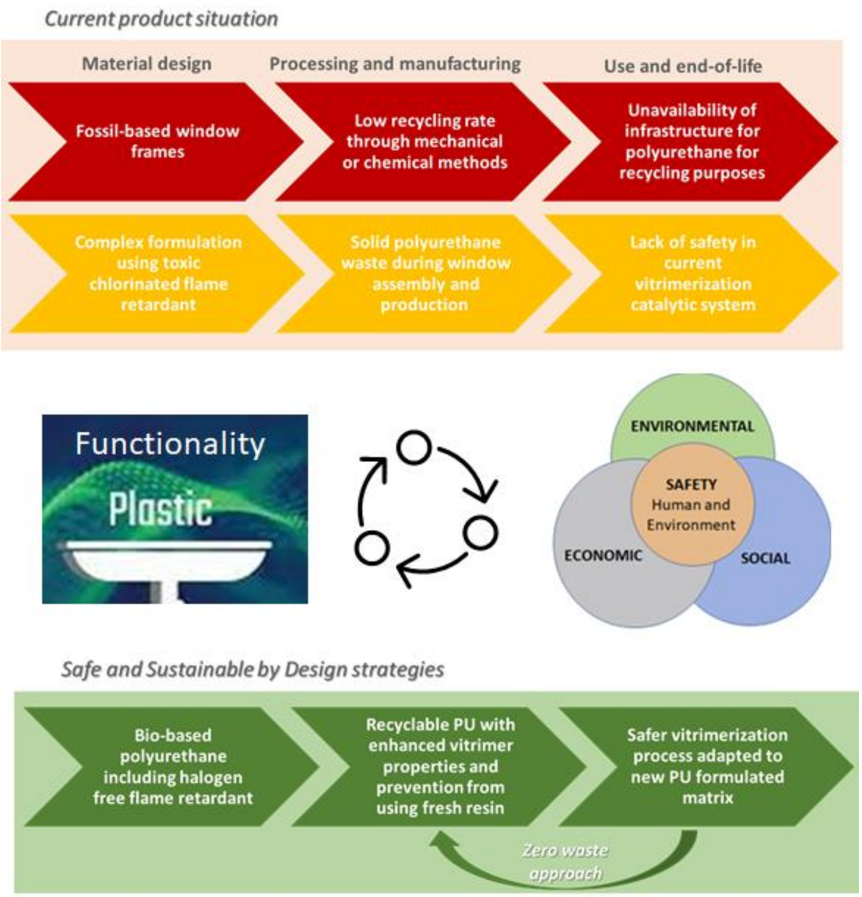


Figure 11. Illustration of balancing functionality with safety and sustainability in an iterative way to obtain safe and sustainable by design strategies + Mapping of the SSbD Approach applied to the Building Case of Study of SURPASS Project

Functionality: Minimal mechanical properties

In here, the functionality concerns the resulting product after the vitrimerization process being a window frame or a similar application. It has been mentioned in the project proposal that CEA, LEITAT and ICT will evaluate performance and compare them to performance metrics of conventional PU material benchmark.

Therefore, the expected minimal properties for a PU window frame can be described as following:

- Mechanical properties: bending strength or flexural strength; defined as the ability to resist deformation under load testing (in D1.2 values from conventional polyurethane material are provided)
- Thermal properties: through thermal analysis such **thermal gravimetric analysis** (TGA) and **differential scanning calorimetry** (DSC)
- **Dynamic thermal mechanical analysis** (DMTA)

  Products reaction to dire:

- Fumes released: International standards such as **ISO 13344, ISO 13571, ISO 9122-4, ASTM E 1678-02, and NFPA 269** have considered various models for estimating the toxic potency of fire effluents. (**reference:** Article Thermal Hazard and Smoke Toxicity Assessment of Building Polymers Incorporating TGA and FTIR—Integrated Cone Calorimeter Arrangement)

Additional information: ISO 19701:2013 Methods for sampling and analysis of fire effluents

https://www.iso.org/ics/13.220.99/x/p/1/u/1/w/0/d/0

- Fire retardancy using safe additives (in this case non-halogenated flame retardants): evaluate their incorporation in the product formulation and their need to succeed specific tests to have ideally A2 classification for fire to reach self-extinguishing properties; according to **UNE-EN 13823:2021** Reaction to fire tests for building products - Building products excluding floorings exposed to the thermal attack by a single burning item, and Reaction to fire tests for products - Non-combustibility test **(ISO 1182:2020)** https://www.fire-testing.com/wp-content/uploads/2020/07/EU-Fire-Testing-Classification-for-Construction-Products_FTT.pdf

Table 8. Functionality: Technical specifications for the development of recyclable bio-based window in the context of the Buildings Case of Study

Insulation properties	**Thermal performance of windows, doors and shutters (ISO 10077-1:2017) — Calculation of thermal transmittance — Part 1: General**	Thermal transmittance window 1040x1040mm = 1,4 W/m2K Thermal transmittance window 1040x1040mm = 1,3 W/m2K
	Thermal transmittance (EN ISO 10077-2:2017 Thermal performance of windows, doors and shutters -- Calculation of thermal transmittance -- Part 2: Numerical method for frames.)	Thermal transmittance of frames/profiles (EN ISO 10077-2:2017) = 0,81 W/(m2K)
	Air permeability (EN 1026:2017 windows and doors: air permeability)	Global classification: Class 3 Classification standard: EN 12207:2017
	Water tightness (EN 1027:2017. Windows and doors: Water tightness)	Global classification: Class 8A Classification standard: EN 12208:2000
Mechanical properties	**Resistance to wind load (EN 12211:2017. Windows and doors. Resistance to wind load)**	Global classification: Class C5 Classification standard: EN 12210:2017
	Resistance to static torsion EN 14609:2004 ERRATUM: 2010. Windows. Determination of resistance to static torsion	Global classification: 350 N CLASS 4 Standard: EN 13115: 2001 Section 4
	Shore A, Shore D hardness test: Standards ISO 48-4/DIN ISO 7619/DIN EN ISO 868/NF EN ISO 868/ASTM D 2240/JISK 6253	Shore D surface = 69 Shore D – 3 mm from surface = 39 Shore D core = 38
	Bend strength: 3 pt bend test, deflection 4 mm Each profile has been bended 3 times with a time interval of 10 mins	Sample: profile INDRESMAT 4mm Machine extension at maximum load = 4,5mm Load at maximum extension = 139,5 N

PU foams are the best and affordable isolation materials present on the market [13]. PU foams have the potential to replace PVC in some building applications, such as the insulating windows frames developed by INDRESMAT.

Material Design

Current situation: fossil-based window frames with complex formulation using toxic chlorinated flame retardant.

Safer solution: Bio-based polyurethane (PU) including halogen-free flame retardant.

INDRESMAT window products are as solid as wooden frames so they do not need metal reinforcement, as for PVC. Besides, these PU foams can be partially **bio-based** (currently <5% w/w bio-based content and a target of more than 75% w/w for the polyol phase by the end of the project). It has proven an extremely high insulating degree, with a heat transmittance more than 2 times lower than that of PVC (CE marking tests results). Its inherent properties allow some hazardous additives to be removed from the formulation, for example **organo-halogen fire-retardant additives** (as used in PVC) that can be efficiently replaced by innocuous mineral nitro-phosphate salts.

Process and Manufacturing re-design

Current situation: low recycling rate through mechanical or chemical methods. Solid polyurethane waste during window assembly and production.

Safer and sustainable solution: recyclable PU with enhanced vitrimer properties and prevention from using fresh resin.

The chemistry of PU makes recycling difficult as it cannot be melt-reprocessed like a thermoplastic. The current solution consists in micronizing unused PU and using it as a filler in new formulations, which allows recycling percentages to be no more than 50%. Yet, less than 30% of thermoset PU is effectively recycled (the remaining is landfilled or incinerated).

Use and End-of-life

Current situation: unavailability of infrastructure for PU for recycling purposes. There is a lack of safety in current vitrimization catalytic system.

Safer and sustainable solution: Safer vitrimization process adapted to new PU formulated matrix resling in zero waste approach.

The SURPASS project will investigate further the use of vitrimer chemistry to increase the recyclability of PU and enable the up-cycling to create a bio-sourced polyurethane resins (PU) with enhanced vitrimer properties to replace Polyvinyl chloride (PVC) for window frames – with similar insulating properties, and able to achieve a higher number of recycling loops.

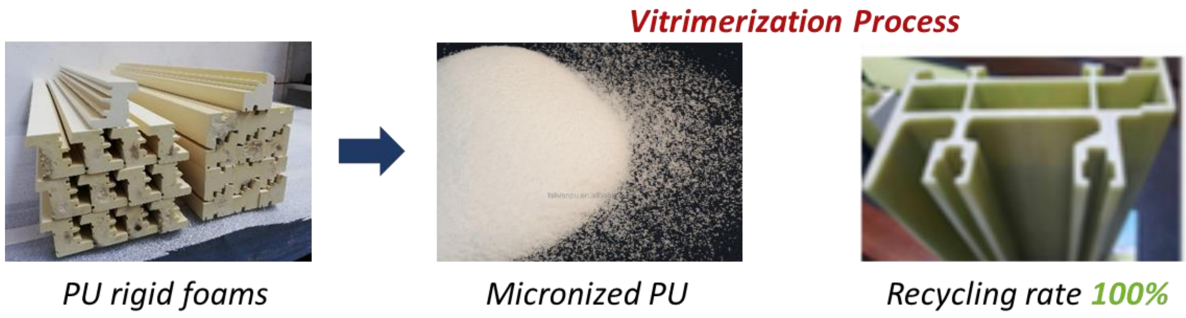


Figure 12. Life stages of PU windows from window frames to 100% recycled material through vitrimerization

Technical approach

Table 9 Identification of life cycle assessments to be evaluated applying the SSbD framework-Building sector Case Study

Life cycle stage	Raw materials sourcing	**INDRESMAT:** bio-sourced polyols, isocyanates, additives (i.e. fire retardants, catalysts, foaming agents, surfactants, UV stabilizers) **CEA:** catalytic system, reactants could be included as well such as cyclic carbonates or amines **LEITAT:** extenders to generate poly(oxime-urethanes)
	Processing	**INDRESMAT:** Formulation of polyurethane matrix **CEA:** grinding rigid foams into a fine powder, impregnation of catalysts using a co-solvent (water or alcohols) **LEITAT:** integration of polyols and extenders in the prepolymer to generate poly(oxime urethanes)
	Manufacturing	**INDRESMAT:** PUR injection process, windows assembly **CEA:** extrusion technology **LEITAT:** compression molding, melt reprocessing loops
	Use	Window installation in buildings
	End-of-life	Window parts separation => mechanical recycling => vitrimerization (reprocessing)

INDRESMAT will adapt its proprietary formulation (proved to be scalable), while working on removable additives to later process it by incorporating the main components, which are the polyol phase and isocyanate phase, in polyurethane injection machine and moulding system to create the window parts.

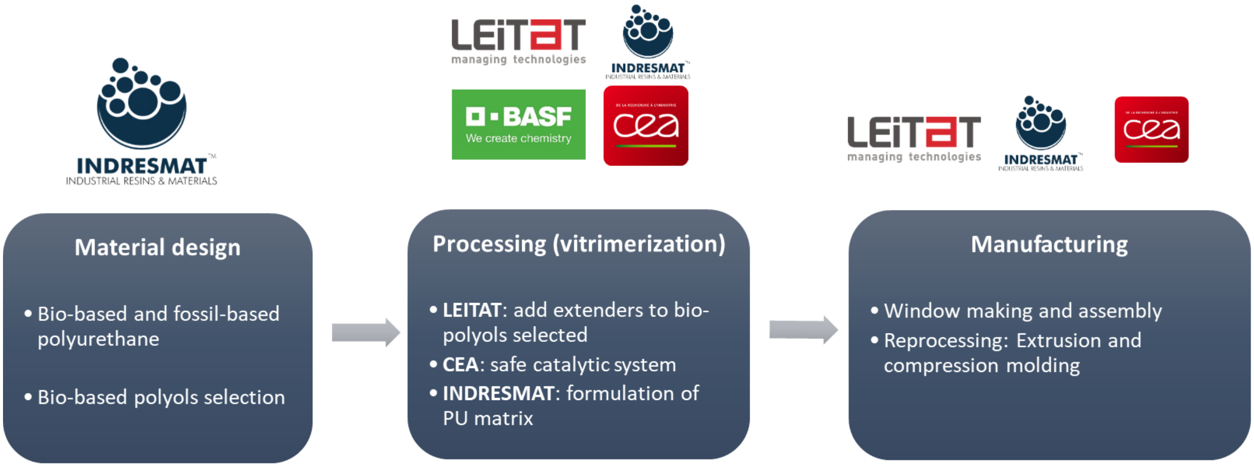


Figure 13. Technical work methodology in case study 1 to obtain recycled and recyclable bio-PU window frames

LEITAT will integrate polyols, selected by **INDRESMAT**, and extenders in the prepolymer to generate new moieties called poly(oxime-urethanes). **LEITAT** aims to modify the INDRESMAT bio-based PU structure through introduction of dynamic chemistry (oxime-carbamate) directly in the PU backbone, thus converting it in a vitrimer, which is reprocessable through compression molding at low temperature.

On the other hand, **CEA** will receive the already commercialized window product and the developed bio-based version, from **INDRESMAT**, to test the vitrimerization feasibility and reprocessability by grinding rigid foams into a fine powder, impregnation of catalysts using a co-solvent (water or alcohols), and then proceed with the extrusion step.

At the end of the SURPASS project, we expect that the reuse of recycled material leads to reducing the use of raw materials for an equivalent mass production (target is of 80-90% of recycled material from classic PU, and 100% recyclability on recycled material). Furthermore, SURPASS aims to be able to reprocess the material continuously within a closed recycling loop. By month 42, the goal is to have developed bio-based window frame formulation, including safe additives, have small scale prototypes produced by LEITAT and 2m length window frame from CEA's side. It is important to mention the contribution of Fraunhofer ICT and BASF in this case study, respectively for the raw materials provision and the polymer characterization and the evaluation of the performances.

4.3.2.3 CS#2 Transport (Epoxy-composite for the railway sector)

Today, metal is still the main material used for the manufacture of structural parts for trains and wagons. The reasons for replacing this heavy material are, on the one hand, the high energy consumption of the manufacturing process and the recycling of the material (very high temperatures) and, on the other hand, the emission of harmful gases due to the significant amount of fuel required for its transport during its life cycle.

In recent decades, the interest in the **use of composite materials** for structural applications for the transport sector has been increasing, mostly because composites are much lighter materials than metal. Currently, in the railway sector, composites are mainly used for interior parts and secondary structures. It is still of great interest to expand the application of these **lightweight materials as alternatives to metals**, which would allow a significant **reduction in vehicle weight** and, thus, **energy**.

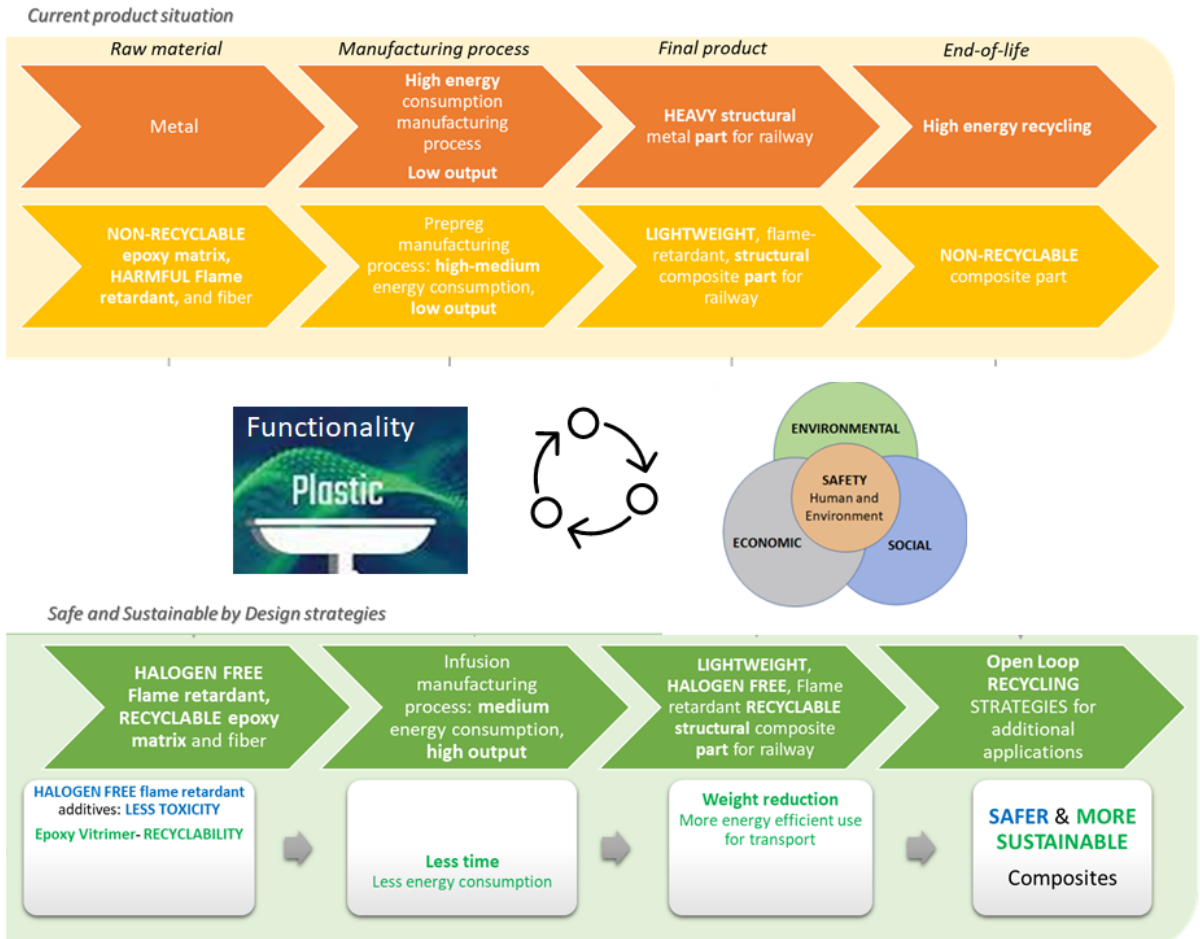


Figure 14. Illustration of balancing functionality with safety and sustainability in an iterative way to obtain safe and sustainable by design strategies + Mapping of the SSbD Approach applied to the Transport Case of Study of SURPASS Project

Minimal mechanical properties

- Fire resistance.
- Fumes released during burning.
- Bending modules.

- Fire resistance through additives using (non-halogenated) which need to pass specific testing; compatible with epoxy resins + safe.
- Mechanical properties (Tg, glass transition temperature; temperature where material is getting softer) defined as the temperature at or above which the molecular structure exhibits macromolecular mobility.
- Traction/flexion testing (classify material) application specific (in D1.2, values from conventional material).
- Hardener is fixed: it gives functionality of recyclability
- Iterative reformulation: at least 110TG or higher; if use fire retardants which are liquid, they shift TG to lower; control concentration of fire retardant to avoid mechanical implications (low TG).
- Working on different epoxy based with fire retardants affect balance of monomer and hardener to keep recyclability.
- Market demand high TG and fire resistance properties; also now recyclability; because becoming big problem (CE).
- Process: production of the part (metal vs composite); composite do not need too high energy.
- Final new composite + flame retardant which is safer (non-halogenated) + sustainable – recyclable + process sustainable (less energy vs metal).

Table 10 Functionality. Technical specifications for the fire-resistant recyclable epoxy vitrimer in the context of the Transport sector Case Study.

Final Product (General information)	**Name**	Fire resistant recyclable epoxy vitrimer for composites	
	Activity Sector	Railway	
Processing properties	**initial viscosity (mPa·s) at working temperature and $10s^{-1}$**	200-320	ISO 3219
	Gel time at specific temperature (min)	infusion (60ºC, $10s^{-1}$): 160 min up to 1 Pa·s [1]	
		RTM (60-80ºC, 1 Hz) <60 (time when G'=G'') [1]	
Mechanical properties (Final Product)	**Glass Temperature (ºC)**	> 110	ISO 11357-2(DSC) ISO 6721-5 (DMA)
	Tensile modulus (MPa)	2860-3350	ISO 527-4
	Tensile Strength at Break (MPa)	> 45	ISO 527-4
	Flexural Strength (MPa)	> 70	ISO 178
Flame resistance (Final Product)	**Hazard level**	HL2[2]	EN 45545-2
	MARHE (kW/m^2)	max. 90	EN 45545-2 ISO 5660-1

	Ds max. (dimensionless)	max. 600	EN 45545-2 ISO 5659-2
	CITG (dimensionless)	max.1.8	EN 45545-2 ISO 5659-2

- [1] *The values shown are for small amounts of pure resin/hardener mix. In composite structures the gel time can differ significantly from the given values depending on the fibre content and the laminate thickness.*
- [2] *Hazard levels are used for material fire safety requirement classifications. There are 3: HL1, HL2 and HL3. (These levels were mentioned in D1.1)*

Material design

Current situation: the use of metal and non-recyclable epoxy matrix which contains harmful flame retardants and fiber.

Safe and sustainable solution: Replacement of toxic flame retardant with halogen-free flame retardant and the use of a recyclable epoxy matrix and fiber.

The application of **composite materials** in rolling stock (primary structures) need to meet specific **fire, smoke, and toxicity (FST) requirements,** which are set by EN45545, to ensure **human and environmental safety**.

The improved **fire resistance** comes from the use of flame retardants (FR) in composite materials. The current trend is to replace halogen-based flame retardants, especially bromine, **with halogen-free flame retardants**, which are **less toxic and more environmentally friendly** [6]**,**[7]. The most common strategies to obtain flame retardant properties in halogen-free epoxy resin formulations are based on the use of inorganic flame retardants such as aluminium hydroxide (ATH), ammonium polyphosphate (APP), various organophosphorus compounds, etc. [7],[8],[9]

Glass or carbon fibre reinforcements for composites have good flame-retardant properties, and therefore it is mainly the resin that needs to be improved in terms of fire resistance.

Recently, some **thermoset composite materials** (i.e. once cured they cannot be re-mixed) that meet the requirements of EN45545 have been developed. However, these novel composite materials are **not sustainable at the end of their useful life**, as they are not intrinsically recyclable, and often end up landfilled or incinerated.

Process and Manufacturing re-design

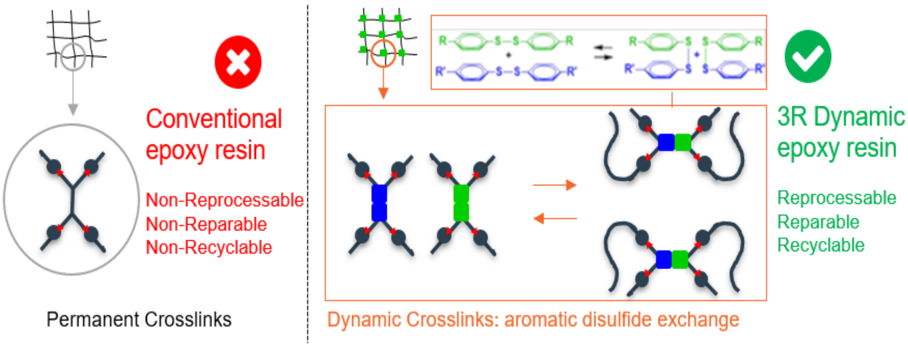
Current situation: The current manufacturing process is energy intensive with low input.

Sustainable solution: Infusion manufacturing process with medium energy consumption and high output.

CIDETEC has developed a sustainable **epoxy vitrimer system** [10] which is easy to synthesize from readily available starting materials in a scalable manner and exhibits rapid high-temperature stress relaxation (vitrimer behaviour) **without the need for a catalyst**, making the **material recyclable**,

reprocessable and repairable (3R) due to the reversible bonds presented in the epoxy vitrimer system on Figure 15.

Figure 15. Schematic representation of conventional epoxy vs recyclable 3R epoxy resin



This vitrimer system is also easily applicable for the manufacture of fibre-reinforced plastic composites (FRPC), giving these composites the ability to also be (re)processable, repairable and recyclable (3R).

Final product re-design

Current situation: heavy structural metal part for railway with lightweight flame-retardant structural composite part of railway.

Safe and sustainable solution: A lightweight, halogen-free flame retardant which is recyclable due to structural composite part of railway.

To anticipate the growing replacement of metal by non-recyclable composite for structures, **SURPASS Case of Study #2**, targeting the transport sector, has the objective of developing **epoxy vitrimers** that:

- meet all the **requirements of the railway FST**;
- achieve the required **mechanical performance**
- fulfil the **needs of the manufacturing process**;
- contribute to **human and environmental safety** through the use of **non-harmful flame retardants** and materials that are intrinsically **recyclable** at the end of their useful life.

End-of-life

Current situation: high energy recycling of the metal and non-recycling composite part.

Sustainable solution: Open look recycling for additional applications.

The rapid stress relaxation behaviour observed in the composites will allow the final product, and the waste generated during production as well, to be recycled through two different routes **in the product's end-of-life** phase. Thus, **recycled parts will be generated**, by simple grinding and thermoforming, and the **epoxy matrix, fibres and flame retardants will be recovered** and used for additional applications.

Technical approach

Table 11. Identification of life cycle stages to be investigated applying the SSbD framework-Transport sector Case study

Life cycle stage	Raw materials	Epoxy resins, hardener components for composites	
		Halogen free flame retardants	
	Processing	Formulation of halogen free flame-retardant epoxy vitrimer (recyclable)	
	Manufacturing	Infusion/Resin transfer moulding (RTM)	
	Use	composites for bogie structure and parts (classified as R7 by EN 45545-2)	EN 45545-2
	End-of-life	Mechanical and chemical recycling to reuse the materials to obtain 2nd generation parts	

The roles of the partners involved in developing this approach are well defined and shown in Figure 16, which also schematically depicts the workflow of this case study.

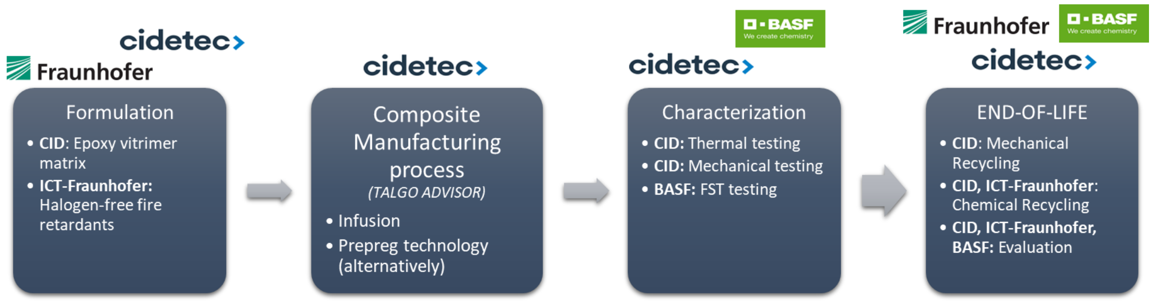


Figure 16 Workflow of the transport case study (railway)

CIDETEC with the support of **TALGO** (member of the Advisory Board) will tackle the manufacturing of composites and evaluate the suitability of the resin system to the manufacturing processing.

CIDETEC in collaboration with **BASF** will carry out the thermal, mechanical and FST testing to evaluate the results and compare them with the technical specification that the material needs to reach to comply with the railway sector requirements.

The recyclability study, at the end-of life stage of the product, will be approached following 2 different routes: mechanical recycling and chemical recycling. **CIDETEC** will address the mechanical recycling by simple grinding and thermoforming. The generated recycled parts, which could be employed for additional applications, will be characterised by **CIDETEC** and **BASF**. Chemical recycling will be carried out by **CIDETEC** in collaboration with **ICT-Fraunhofer**. The resin will be completely dissolved, and the reinforcement will be recovered undamaged through an exposure to a specific chemical reagent, which will enable the exchange bonds with the dynamic network. The resin and the fire-retardant additive can also be recovered and re-used for other applications.

4.3.2.4 CS#3 Packaging (Recyclable Multi-nanolayered films to replace multi-layer films for food packaging with drastically reduced concentrations of compatibilizers)

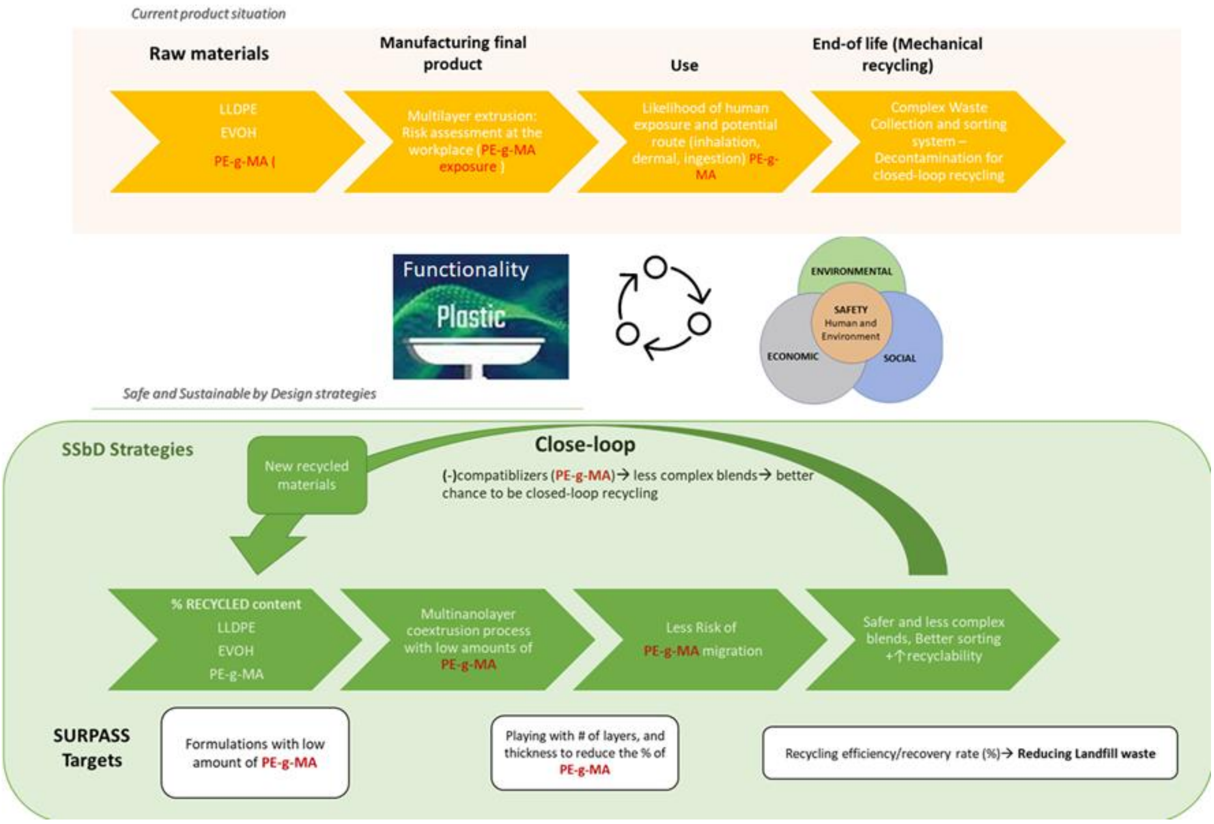


Figure 17. Illustration of balancing functionality with safety and sustainability in an iterative way to obtain safe and sustainable by design strategies + Mapping of the SSbD Approach applied to the Packaging Case of Study of SURPASS Project.

Minimal mechanical properties

- Sealability, printability and resistance against abrasion.
- Oxygen barrier.
- Shelf-life.
- Sealing strength.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement N°101057901

Table 12 Functionality. Technical specifications for the design of Multi-nanolayers films in the context of the Packaging Case of Study

Final Product (General information)	Name	Multilayer film
	Activity Sector	Food Packaging
	Product Lifetime	Shelf life multilayer film up to 2 years - shelf life for product packed can be up to 6 months depending of product
General Characteristics of final product	Width (mm)+tolerance	422 (0 +1)
	Thickness (µm)+tolerance	200 (+/-10%) - other options possible in range 50 to 300 µm
	Food contact layer	LLDPE (External layer)
	Shrinkage (%)	MD/TD = < 10%,
	Indicative values(directly after thermoforming)	additional shrinkage (after 24h package) MD/TD = < 5%
	Thermoforming range (indicative) (°C)	90°C to 110°C
Mechanical properties (Final Product)	Young's Modulus (N/mm²) MD	350 (method based on ASTM D882)
	Young's Modulus (N/mm2) TD	400(method based on ASTM D882)
	Tensile Strength at Break (N) MD	> 65 (method based on ASTM D882)
	Tensile Strength at Break (N) TD	> 65 (method based on ASTM D882)
	Elongation at Break (%) MD	> 400% (method based on ASTM D882)
	Elongation at Break (%) TD	> 400% (method based on ASTM D882)
	Seal Strength (N/m)	> 1200 (method based on ASTM F88)

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement N°101057901

Material Design

Current situation: External layers of Polyolefins as low-density polyethylene (LDPE) with EVOH (Ethylene and Vinyl Alcohol copolymer) for barrier properties. Unfortunately, most current designs and the absence of sorting and recycling technologies for such multilayers make them unsuitable for recycling in an economically and environmentally sustainable way.

Safe and sustainable solutions: PE/EVOH and PE/PA blends are developed to form base multilayer films without multipliers.. The Multi-nanolayer (MNL) polymer based films result in low PE-g-MA blends.

Multilayer plastic films are widely used as packaging for food protection and preservation. Thanks to their unique barrier properties, protection can be provided directly by preventing goods from contamination and indirectly by extending its shelf life [14].

The Multilayer films are commonly composed by multiple high performance layers, each one having their own useful function. Regardless their design, the outer layer provides sealability, printability and resistance against abrasion. Meanwhile, the inner layer provides oxygen barrier properties. The most common materials used for the external layers are the Polyolefins as low-density polyethylene (LDPE) being the most prominent, followed by polypropylene (PP), high-density polyethylene (HDPE), and polyethylene terephthalate (PET). As regards the barrier properties, PA (polyamide), EVOH (Ethylene and Vinyl Alcohol copolymer), are widely used. PE/EVOH and PE/PA blends are developed to form base multilayer films without multipliers. The Multi-nanolayer (MNL) polymer based films result in low PE-G-ma blends.

Process and Manufacturing re-design

Current situation: Multi-layer extrusion where risk assessment is necessary at the workplace to ensure there is minimal PE-g-MA exposure. Pe-g-MA is irritating to the eyes, the respiratory system and the skin[3].

Safe and sustainable solution: multi-nanolayer coextrusion process with low levels of PE-g-MA. Playing with the # of layers and thickness to reduce the % of PE-g-MA.

Multi-nanolayer films coextrusion in SURPASS Project: Within the scope of SURPASS, IPC will first establish combinations of PE/EVOH and PE/PA blends, with the support of WIPAK and BASF, to form base multilayer films without multipliers, This step is needed to test the homogeneity of the layers and their interfacial adherence, as well as for optimizing the viscosity difference between the co-extruded polymers. These films will serve as a reference for the specific Case of Study.

Afterwards, IPC will formulate blends with different concentrations of compatibilizers applying the multi-nanolayer coextrusion technology, using diverse multiplying elements. The objective is to obtain

[3] POLYETHYLENE-GRAFT-MALEIC ANHYDRIDE CAS#: 106343-08-2 (chemicalbook.com)

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multi-nanolayer films with up to 1024 layers. Therefore, with the best formulations, IPC will investigate the influence of the nanolayering parameters (number of layers, thickness, and composition of the layers) on the barrier and mechanical properties of the final product.

Use and End-of-life

Current situation: likelihood of human exposure (via inhalation, dermal and ingestion) to PE-g-MA. Pe-g-MA is irritating to the eyes, the respiratory system and the skin[4]. There is also a complex waste collection and sorting system needing decontamination for closed look recycling.

Safe and sustainable solution: Safer and less complex bends resulting in better sorting, increased recyclability and reduction of landfill waste; all supporting a closed material loop recycling.

[4] POLYETHYLENE-GRAFT-MALEIC ANHYDRIDE CAS#: 106343-08-2 (chemicalbook.com)

Technical approach

Table 13. Identification of life cycle assessments to be evaluated applying the SSbD framework-Packaging sector Case Study

<table>
<tr><td rowspan="7">Life cycle stage</td><td rowspan="2">Raw materials</td><td>Material</td><td>LLDPE</td><td>EVOH</td><td>PA6</td><td>PE-g-MA</td></tr>
<tr><td>Function</td><td>External layer</td><td>Barrier layer</td><td>Barrier layer</td><td>Tie-layer (Compatibilizer)</td></tr>
<tr><td>Processing (raw materials)</td><td>Material</td><td>LLDPE</td><td>EVOH</td><td>PA6</td><td>PE-g-MA</td></tr>
<tr><td></td><td>Polymerization Process</td><td>Low Pressure</td><td>High pressure</td><td>Polycondensation</td><td>Reactive modification of PE - Grafting reaction Co-Polymerisation</td></tr>
<tr><td colspan="2">Manufacturing (final product)</td><td colspan="4">Multi-nanolayer extrusion process</td></tr>
<tr><td colspan="2">Use (final product)</td><td colspan="4">Barrier films for food packaging applications (e.g. thermoforming films for cheese bloc, or meat with/without bones, fish as salmon…)</td></tr>
<tr><td colspan="2">End-of-life (final product)</td><td colspan="4">Mechanical recycling to integrate PE stream -Close loop (Food packaging)</td></tr>
</table>

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement N°101057901

The roles of the partners involved in this case of study are well defined and shown in

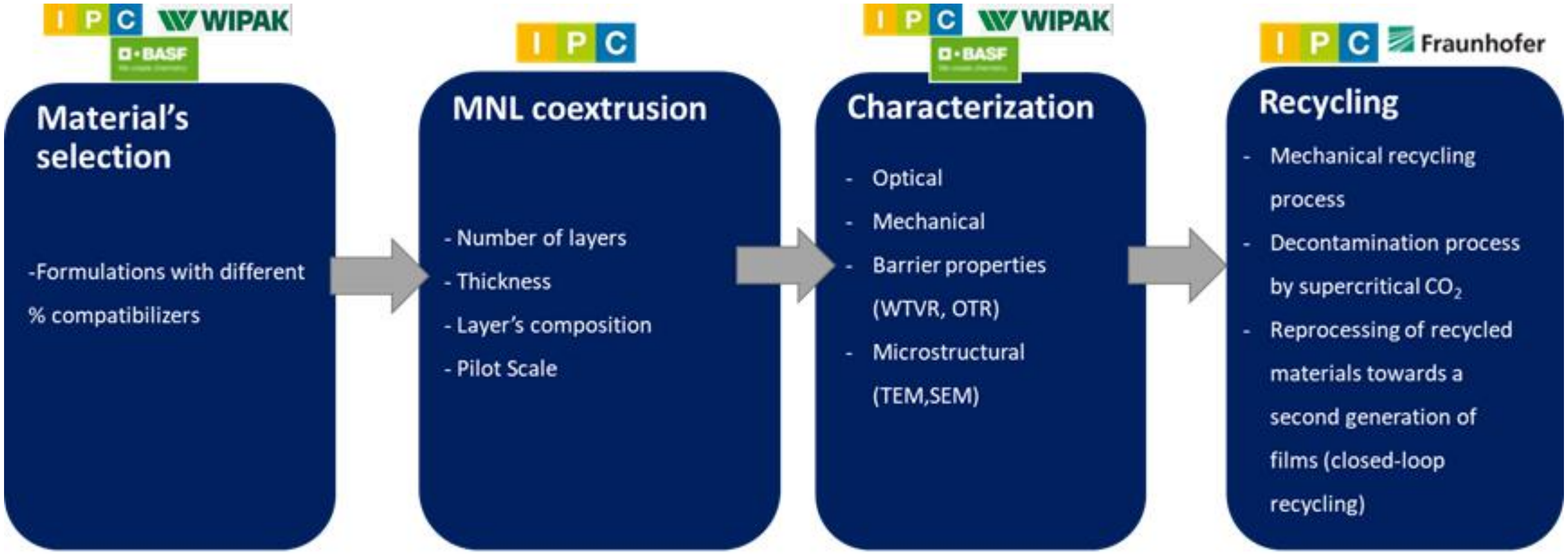

Figure 18. It schematically depicts the workflow of this case study which will be carried out in SURPASS Project.

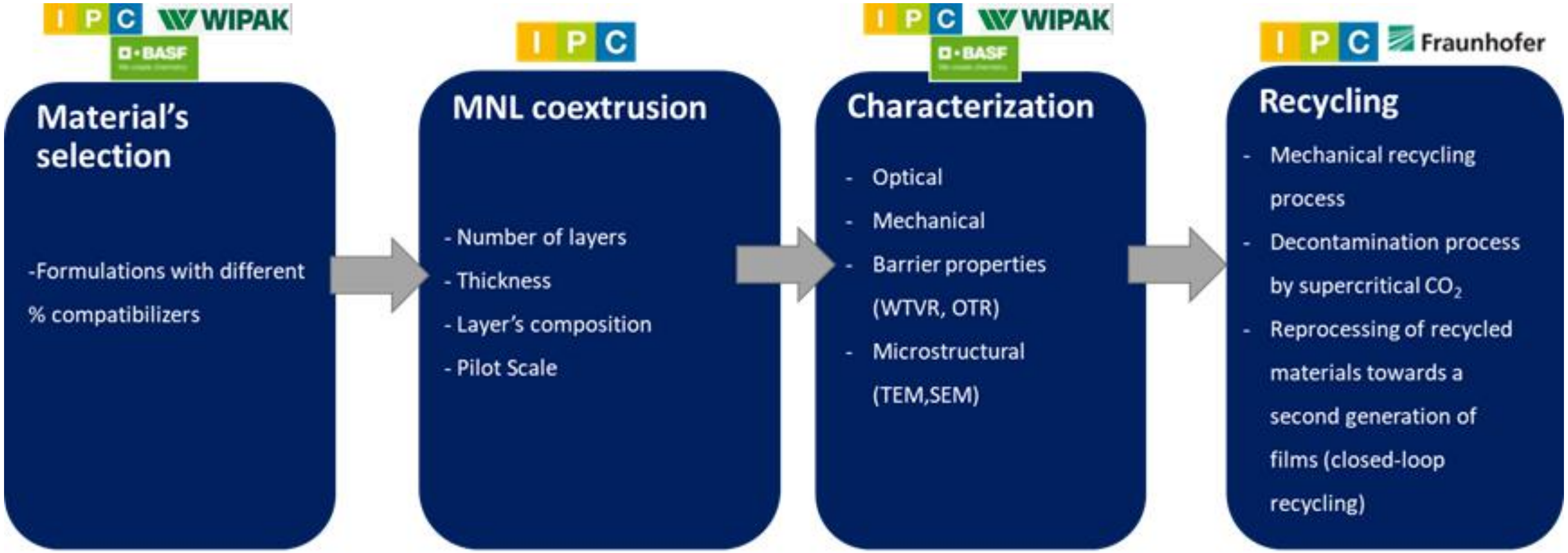

Figure 18. Workflow of the Packaging case of study

4.4 Verification of Safe-Sustainable-and-Recyclable-by-Design strategies to ensure they lead to safer and more sustainable alternatives (Step 3, Towards an integrated SSRbD approach)

In order to verify the SSRbD Strategies, Table 14 provides a general guidance on what polymer material information needs to be collected for the dimensions of safety, sustainability, functionality and economic across the various stages of material, product and process. The data presented in Table 14 and that collected Section 5 will be translated into a dashboard which allows monitoring of the progress of safety and sustainability early in the innovation process by displaying the current and target baselines for the areas of management and results through several radar diagrams for the considered period. There is a main dashboard composed of 1. Functionality, 2. Safety, 3. Environmental Sustainability, 4. Economic Sustainability, and 5. Social Sustainability. The basis of the SURPASS dashboard is the CEN CWA 17935 (Sustainable Nanomanufacturing Framework) (See Section 5 for further details).

Table 14 Guidance for identifying polymer material relevant information needs for the dimensions of safety, sustainability, functionality and economic across the various life stages of polymeric materials, product and process.

Functionality	Safety (human and environmental) aiming at minimize human health and environmental impacts (T4.2 & T4.3) [2, 15-17].	Environment (T4.4) aiming to minimizing the environmental footprint [2, 17-22].	Economic (T4.5) aiming at optimizing economic feasibility and value [16-20, 22].	*Social aiming to improve the social aspects (worker, local communities, consumers and society as a whole)* [17-20, 22, 23] *(not covered in SURPASS yet important elements identified)*
Transport (rail) - Fire resistance through the addition of additives and/or resin modification. - Mechanical properties (**Tg**, glass transition temperature - temperature where material becomes softer-, **tensile** and **flexural** properties) -Recyclability by vitrimerization	Exposure characterization / assessment (T4.2) - What is the intended formulation and the potential exposure route and population? - Which transformations of the polymeric material can be expected throughout the life cycle?*** - Which types of exposure and release scenarios can be expected? Qualitative description of intended material production process, product production and after use. - Occupational exposure measurement (measures workers exposure concentrations. - What are relevant exposure reduction measures? Assessment of relevant	Raw Materials and resources - Are critical raw materials^ used? - Does the process of extracting the raw materials require high energy, water, or land consumption and/or have an environmental impact? - Can recycled material be used to replace raw materials Manufacturing - Does the manufacturing process require high energy, water, or land consumption and/or have an environmental impact? - Can the manufacturing process be energy and water efficient? - Is there a high amount of waste in the process of manufacturing?	- Is there expected profitability (Social and economic value, net present value, financial profit, payback period)? - What are life cycle cost & externalities? - Does polymeric material and product meet market-related criteria (Meeting stakeholder expectations and product performance)? - Is there transparency and information about polymeric material and product? - What is the product cost (purchase cost, production cost)?	- *Is customer protection (health & safety of local community's living conditions, product safety, impact on consumer health) considered?* - *Is Occupational health & safety Health & Safety (occupational health risks, safety management a work, management of worker's individual health, (see safety – human) considered?* - *Human and Labor rights/Basic rights & needs (fair wages, appropriate working hours, no forced labor, human trafficking and slavery, no discrimination, harassment prevention,*

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement N°101057901

Functionality	Safety (human and environmental) aiming at minimize human health and environmental impacts (T4.2 & T4.3) [2, 15-17].	Environment (T4.4) aiming to minimizing the environmental footprint [2, 17-22].	Economic (T4.5) aiming at optimizing economic feasibility and value [16-20, 22].	*Social aiming to improve the social aspects (worker, local communities, consumers and society as a whole)* [17-20, 22, 23] *(not covered in SURPASS yet important elements identified)*
Construction (window frames) -Fire retardancy -Fumes released during burning -Bending strength or flexural strength -TG (glass transition temperature),DSC - DMTA Food packaging - Sealability, printability and resistance against abrasion - oxygen barrier - Shelf-life - Sealing strength	exposure reduction measures and their efficiency. - What is the outcome of the risk assessment of the polymeric material for the relevant exposed populations throughout the life cycle of the product? What are the uncertainties in this assessment? Are there still important data gaps (e.g. advice for further testing)?[####] - Does occupational exposure increase due to the upscaled process? Update of relevant exposure reduction measures in occupational setting in response to up scaling. - Is the quality of the production process sufficient? - Mobility/Public health exposure considerations? Hazard characterization/assessment (T4.3) Human toxicity: - Are the raw materials used classified as hazardous or persistent (CLP)?[^^] (Avoid the use of hazardous or persistent substances, as they may circulate or hamper the re-use potential of materials or products). - Are there any hazardous properties identified in REACH, CLP? Is there any Ecotoxicological (potential accumulation/persistency) information (e.g. basic information on potential ecotoxicity, read across data) in scientific literature? How are the chemical components labelled? Are there any CMRs, ED or SVHC**?	- Is the waste generated during manufacturing recyclable or reusable? - Does the emissions or waste generated during manufacturing contain persistent or hazardous substances (CLP)? - In the processes of manufacturing, what volume of solvents or water are used? Production, - Does the production process require high energy, water, or land consumption and/or have an environmental impact? - Can the production process be energy and water efficient? Opportunity of relocation of manufacturing where energy and water efficiency is improved: less transport, better energy carbon footprint? - Is there a high amount of waste in the process of production? - Is the waste generated during production recyclable or reusable? - Does the emissions or waste generated during production contain persistent or hazardous substances (CLP)? - In the processes of production, what volume of solvents or water are used? Transport - Does the transportation process require high energy, water, or land consumption and/or have an environmental impact? - Is there a high amount of waste in the process of transportation? - Is the waste generated during transportation recyclable or reusable? - Does the emissions or waste generated during transportation contain persistent or hazardous substances (CLP)?	- Is there value chain collaboration to ensure lifecycle thinking approach? - Are circular business models used? - Is essentiality information available?	*social/employer security and benefits, access to basic needs, respect for human rights and dignity).* - *Supply chain responsibility, (community engagement, local employment, safe and healthy living conditions, transparency and responsible communication, consumer product experience, end-of-life responsibility)* - *What is the contribution to economic and technology development (education, job creation, joint research)?* - *Skills & knowledge (skills, knowledge and employability, promotion of skills and knowledge for local community and consumers)*

Functionality	Safety (human and environmental) aiming at minimize human health and environmental impacts (T4.2 & T4.3) [2, 15-17].	Environment (T4.4) aiming to minimizing the environmental footprint [2, 17-22].	Economic (T4.5) aiming at optimizing economic feasibility and value [16-20, 22].	*Social aiming to improve the social aspects (worker, local communities, consumers and society as a whole)* [17-20, 22, 23] *(not covered in SURPASS yet important elements identified)*
	- Are there any legislative restrictions associated with polymeric material? - Characterisation of polymeric material: - Polymer class - Polymer type - Grade - Additives - Blends - Production residues - Non-intentionally added substances (NIAS) - Is the polymeric material bio-persistent? - What is the toxicity of the polymeric material (if *in vitro* and *in vivo* toxicity test are performed)* - For transformation and recycling process: Are there any restricted or toxic process contaminant? - Which transformations of the polymeric material can be expected throughout the life cycle?*** - Is it possible to use read across or grouping of relevant forms to fill remaining data gaps for risk assessment?### Environment toxicity - Ecotoxicity: Are there any legislative restrictions REACH, CLP associated with polymeric material? - Ecotoxicological (potential accumulation/persistency) information (e.g. basic information on potential	Use - Does the use require high energy, water, or land consumption and/or have an environmental impact? - Is there a high amount of waste in the process of manufacturing? - Is the waste generated during use recyclable or reusable? - Does the emissions or waste generated during use contain persistent or hazardous substances (CLP)? - During use, what volume of solvents or water are used? End-of life (Recyclability and reusability) - Can the raw material in the application context be recycled, re-used or recovered? - Is the recycling process efficient? (i.e. is volume and quality of recycling product sufficient for a circular economy?) - Is there an efficient system in place to recycle the products? Or is there a concept or plan to recycle the material/recover the individual materials? - Does the process of recycling require high amounts of energy, water, or land consumption and/or have an impact on global warming potential (emission of greenhouse gases)? - Is it possible to re-use (most of) the materials in the same or another function? - Are different components used that are integrated, which might make recycling technically difficult? - Is the application of the material or product durable e.g. long-term functionality, or		

Functionality	Safety (human and environmental) aiming at minimize human health and environmental impacts (T4.2 & T4.3) [2, 15-17].	Environment (T4.4) aiming to minimizing the environmental footprint [2, 17-22].	Economic (T4.5) aiming at optimizing economic feasibility and value [16-20, 22].	*Social aiming to improve the social aspects (worker, local communities, consumers and society as a whole)* [17-20, 22, 23] *(not covered in SURPASS yet important elements identified)*
	ecotoxicity, read across data) in scientific literature. - Ecotoxicological information (specific information on potential acute & chronic ecotoxicity, potential bioaccumulation. - *In vivo* acute & chronic ecotoxicity test on algae, crustacean and fish Ecotoxicological information: Growth inhibition in aquatic plants, In vitro tests using relevant cell lines: cytotoxicity assays for metabolic activity, membrane integrity, lysosomal function. Biopersistency and biodurability.	reparable? (Durable indicates that there is long-term functionality) Other aspects - Protection & restore biodiversity and ecosystems services. - Other relevant indicators that might be considered abiotic depletion, acidification, eutrophication, ozone layer depletion, photochemical oxidation potential, particulate matter (respiratory inorganics), ionizing radiation (effects on human health)		

CLP , Classification, labelling and packaging; C&L Inventory - ECHA (europa.eu)
*Toxicity, CLP of polymeric material
**CMR, Carcinogenic, mutagenic and reprotoxic; ED, endocrine disruption; SVHC, Substance of very high concern
*** Physicochemical properties of the polymeric material throughout the life cycle of the product.
**** Please, select the most important endpoints based on expected exposure.
# Exposure scenarios of hotspots throughout the production process and downstream use of the products, including waste disposal (theoretical information).
Please, select the most important endpoints based on the expected exposure.
Earlier obtained information for read across or grouping as described in the ECHA guidance (i.e. phys-chem and in vitro data of relevant polymeric materials and phys-chem and hazard information of similar polymeric materials) [24].
Earlier obtained information for the risk assessment of all relevant polymeric materials for all relevant exposure scenarios (e.g. exposure quantities of relevant exposure scenarios and hazard information on relevant or similar polymeric materials)
^Critical raw materials (europa.eu)
^^CLP Legislation - ECHA (europa.eu)

5 Overview of information needs for the application of SSbD

In order to develop a dashboard to aid in the application of SSbD early in the innovation process, information needs were mapped according to:

1. General information needs,
2. Release and exposure,
3. Health and environmental impact assessment, and
4. Life cycle costing

As explain at paragraph 4.3, the TRL levels of the CSs range from 3 to 5 and to operationalise the assessment, a tiered approach with the realisation of three assessment loops was chosen. The loops are early in the innovation process, mid in the innovation process and late in the innovation process. Information needs and indicators are listed according to these three tier.

Table 15. General information needs mapped to the innovation process

Information needs	Early in the innovation process	Mid in the innovation process	Late in the innovation process
Map known value chain-specific issues	X		
Criticality (are critical materials used?)*	X		
Characterisation of polymeric material: • **Polymer class** • **Polymer type** • **Grade** • **Additives** • **Blends** • **Production residues** • **Non-intentionally added substances (NIAS) : pollutant/contaminant, degradation product etc.**	X**		
Recycling and processing data (energy/water consumption, waste, production, etc)		X	

*Raw Materials Information System (europa.eu)
**For hazard assessment, it is essential to know the raw materials early in the innovation process. This gives the manufacturer the option to substitute to a safer alternative if available.

The needs depend on the process maturity, from early to late via mid. Depending on the process maturity, the assessment time and complexity should be adapted. An early (low data, time and

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complexity) assessment is performed for all the possibilities developed in the case studies. Once the maturity of the process is enhanced to several possibilities, a mid assessment is performed. The late (complex, lot of data, time-consuming) assessment is performed only on the final hot spots.

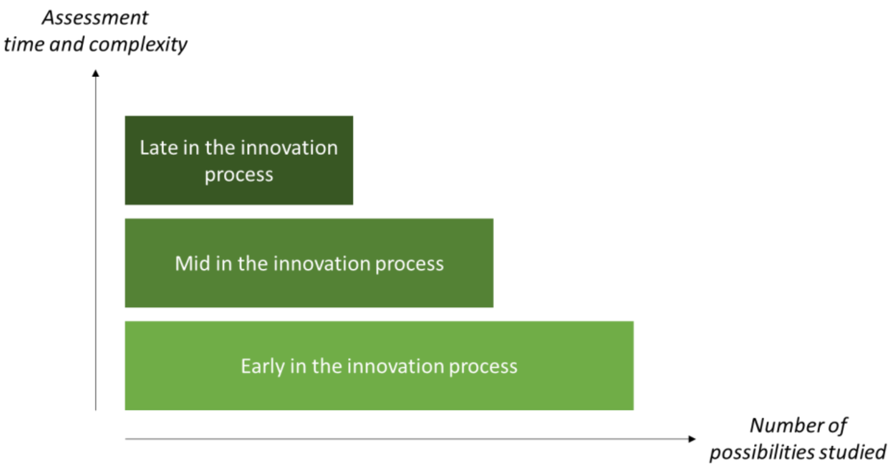

Figure 19. Three SSbD levels are available depending on the process maturity

5.1 Hazard

5.1.1 Overview of information needs

As a first step, the individual components of the product need to be identified as listed in Table 16. These provide the basis for the hazard assessment. Starting with the bulk components, available hazard information can be gathered from ECHA. All chemical substances that are being produced or imported into the EU need to be registered and there hazard information is available at the website of ECHA. For each component of the product, the ECHA database can be used to identify whether components are classified for a specific hazard. Based on available classification information, components can be considered a substance of very high concern (SVHC), and thus prioritized for substitution.

For some substances, there might be sufficient information available while for other substances there can be data gaps. Based on information on exposure and release, substances can be prioritized for filling the hazard data gaps. Data gaps can be filled by searching open literature and by applying in silico modelling such as QSAR to identify if specific chemical structures raise a hazard alert. If these searches do not provide sufficient information, additional toxicity testing might be considered. Testing will start using relatively simple in vitro methods. For some toxicity endpoints, standardized in vitro assays are available that could be used early in the innovation process. For other endpoints including reproductive toxicity and carcinogenicity, animal studies might be necessary prior to market entrance. Only in case a product is late in the innovation process and close to the market, animal testing could be considered to fill a data gap for the risk assessment.

A special case is the endpoint of endocrine disruption. Endocrine disrupting chemicals are considered of high concern. However, there is no consensus which assays and testing are sufficient to classify a chemical as being ED. Screening for potential ED within a SSbD context is therefore very challenging.

Table 16. Hazard information needs mapped to the innovation process.

Information needs	Early in the innovation process	Mid in the innovation process	Late in the innovation process
Hazard assessment (intrinsic properties)			
Identification of additives metabolites and their detoxification kinetics	x		
Physical hazard: Physical properties	x		
Human health hazard			
CLP / SVHC / PMT	X		
Cytotoxicity	X		
Inflammation	x	X	
Oxidative stress	X	x	
Genotoxicity	X		
Epigenetic damage			
Endocrine disruption (ED)	X		
Acute human health		X	
Chronic human health		x	X
Process-related hazards (processing and recycling)		X	
Human health and safety aspects of production and processing			
Human health aspects in the final application phase			
Human health aspects in the end-of-life treatment (between end-of-life and recycling)			
Environmental hazard			
CLP / SVHC / PMT	X		
Ecotoxicity	x	X	X
Environmental safety aspects of production and processing			
Environmental aspects in the final application phase			
Environmental aspects in the end-of-life treatment (between end-of-life and recycling)			

Table 17 Overview of relevant hazard frameworks

Number	URL	Recommended by	Reasons for recommendation	Highlighted features	Description of framework
1	ECHA DNEL Guidance Document (Part B)	Rubén Álvarez (LEITAT)	Widely used / accepted	· Determination of Derived No-Effect-Levels (DNELs) (Part B, Chapter R.8). ·Determination of Predicted No-Effect-Concentrations	Part B of "the guidance on information requirements and chemical safety assessment" covers the information that must be provided in the CSA in terms of hazard assessment. This CSA is only

				(PNECs) (Part B, Chapter R.10).	required under REACH framework for those substances which a REACH registration dossier is required and covers a tonnage band above 10 t/y.
2	ECHA CLP Guidance	Rubén Álvarez (LEITAT)	Widely used / accepted	Guidance to Regulation (EC) No 1272/2008 on classification, labelling and packaging (CLP) of substances and mixtures.	Guidance on application of the CLP criteria.
3	Test Methods for phys-chem properties for REACH registration	Rubén Álvarez (LEITAT)	Widely accepted	Test methods to determine the physicochemical properties, toxicological and ecotoxicological endpoints which are required to submit a REACH registration dossier.	COUNCIL REGULATION (EC) No 440/2008 of 30 May 2008 laying down test methods pursuant to Regulation (EC) No 1907/2006 of the European Parliament and of the Council on the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH).
4	Regulation (EU) 1907/2006 (EU REACH) (Annex XIII)	Rubén Álvarez (LEITAT)	Consolidated version	Criteria for identification of PBT and vPvB · Screening and assessment of P, vP, B, vB and T properties.	Annex XIII of REACH Regulation describes all relevant information for the determination of PBT properties of a substance.
5	Commission Delegated Regulation (EU) 2023/707	Rubén Álvarez (LEITAT)	It came into force recently.	New CLP categories: ED, PMT / vPvM.	Amendment of Regulation (EC) nº 1272/2008 (CLP Regulation), which came into force on 20 April 2023.

5.2 Release and exposure

5.2.1 Overview of information needs

Information on possible release hotspots of materials along the life cycle of the investigated materials need to be collected considering guidelines and protocols developed by European Authorities (e.g., ECHA and OECD). As a first step, a list of all the substances used for each activity performed in each life cycle stage need to be collected with the hazard information according to the ECHA database. In parallel, a list of potential targets exposed (i.e., workers, consumers, general population and environment) and route of exposure/environmental compartments are considered as a starting point to identify vulnerable targets. Then, specific information related to the targets (e.g., level and type of containment used) need to be collected following the ECHA guidelines listed in paragraph 5.1.2.

Degradation and transformation processes (e.g., changing of tensile strength, colour, molecular weight) of the polymers can be investigated by developing a chemical inventory of the released/degraded forms from the polymeric materials used along the entire life cycle. Information gathered from a literature search as well as from experimental tests can help in this purpose.

Table 18 Release and exposure information needs mapped to the innovation process

Information needs	Early in the innovation process	Mid in the innovation process	Late in the innovation process
Overview of LCS, process and activities in which a certain material is/will be used	x		
Release and exposure foreseen (making use of simple exposure assessment models)?	x		
High energy activity/ is present/foreseen?	x	x	x
Type(s) of material(s)/ product(s) used and their physicochemical form	x	x	x
Where the processes/ activities will take place	x		
Risk mitigation measures and/or personal protective equipment used?	x	x	x
Who is performing the processes/ activities?	x	x	x
Which are the (potentially) exposed population(s)?	x	x	x
Which are the (potential) exposure routes?	x	x	x
In which compartment(s) are the material(s) released?	x	x	x
Chemical Hazards from release behavior in processing and recycling step		X	

5.2.2 Overview of the relevant frameworks

Table 19 Overview of relevant release and exposure frameworks

Number	URL	Recommended by	Reasons for recommendation	Highlighted features	Description of framework
1	Guidance on Information Requirements and Chemical Safety Assessment (R.12 - Use description)	Camilla Delpivo (LEITAT)	Widely used	Use scenarios	
2	Guidance on Information Requirements and Chemical Safety Assessment (R.14 - Occupational Exposure Assessment)	Camilla Delpivo (LEITAT)	Widely used/ accepted	Consumer exposure assessment	
3	Guidance on Information Requirements and Chemical Safety Assessment (R.15 - Consumer Exposure Assessment)	Camilla Delpivo (LEITAT)	Widely used/ accepted	Occupational exposure assessment	
4	Guidance on Information Requirements and Chemical Safety Assessment (R.16 - Environmental Exposure Assessment)	Camilla Delpivo (LEITAT)	Widely used/ accepted	Environmental exposure assessment	
5	Guidance on Information Requirements and Chemical Safety Assessment (R.18 - Exposure scenario building and environmental release estimation for the waste life stage)	Camilla Delpivo (LEITAT)	Widely used/ accepted	Exposure scenario building and environmental release estimation for the waste life stage	

5.3 Health and environmental impact assessment

The innovative CS implemented in the Surpass project occur in a complex industrial system. To facilitate the health and environmental impact assessment, a global practical approach to support the development of the SSRbD strategy is presented in section 4.3.2.1. The health and environmental impact assessment will be carried out during the evaluation step following the JRC framework. A complex system industry is characterised by large size and mass, and relatively long and uncertain life cycles. The associated organisation is also complex, as there are many highly specialised experts who rarely work together, and even less so on environmental aspects [25]. The strategy to operationalise the Health and environmental impact assessment as presented in introduction of paragraph 5 is to apply a tiered approach where different levels of assessment could be conducted. Depending on the development levels of the product (Early, Mid and Late), the tool used could be different (Table 20).

Table 20 Health and environmental impact assessment tools needs mapped to the innovation process

Early in the innovation process	Mid in the innovation process	Late in the innovation process
Life cycle Design Strategy wheel	LCI with a resource and environmental profile analysis (REPA) Hot spot screening with LCA	Complete application of the LCA methodology

5.3.1 Overview of information needs

The development of innovative plastics is usually driven by technological limitations and regulations and does not always take environmental issues into account. In addition, the complexity of new product development and organisation makes it difficult and time consuming to integrate health and environmental impact assessment into the company's management system. The Table 21 summarises the information needs according to the stages of product development. So early in the innovation process, the health and environmental impact assessment should be based on qualitative answers to a minimum number of questions based on the 8 SSbD principles. At mid-term in the innovation process, the information to feed the SSbD principles can be quantified, using value ranges, in a screen life cycle inventory. It may not necessarily cover the whole product life cycle but it is needed for a preliminary identification of health and environment hotspots and possibly carry out a resource and environmental profile analysis. This aims at identifying pathways for eco-design options to be implemented and further assessed. At the late-stage in the innovation process, a comprehensive LCA is needed to assess the health and environmental impacts. Based on a comprehensive life cycle inventory, covering the whole life cycle, this assessment provides quantified information on health and environment impacts, through a number of impacts categories that are defined by characterization methods and provide quantified indicators of impacts. The LCA methodology is mainly based on standards (Table 22). For a more comprehensive presentation of the LCA methodology please refer to Deliverable D4.5. At this late stage of the innovation process, the level of uncertainties for impacts values is lower. Hotspot identification is more reliable but the freedom for further eco-design developments is then reduced.

Table 21. Health and environmental impact assessment information needs mapped to the innovation process.

Information needs	Early in the innovation process	Mid in the innovation process	Late in the innovation process
Based on a qualitative questionnaire	**X**		
Based on a quantitative questionnaire		**X (value ranges)**	**X (specific values)**
Material efficiency (SSbD1)	X	X	
Use of hazardous chemicals (SSbD2)	X	X	
Design for energy efficiency (SSbD3)	X	X	
Use of renewable resources (SSbD4)	X	X	
Hazardous emissions (SSbD5)	X	X	
Exposure to hazardous substances (SSbD6)	X	X	
Design for end-of-life (SSbD7)	X	X	
Life cycle perspective (SSbD8)	X	X	
Based on data collection for goal and scope definition		**X**	**X**
Product description, including function		X	X
Life cycle stages to consider		X	X
Product application field			X
Methodology to be applied			X
Based on data collection for inventory		**X**	**X**
Material, water and energy consumptions		X	X
Waste generation (nature and fate)		X	X
Emissions (to air, water and soil)		X	X
Based on screen LCA		**X**	
Based on comprehensive LCA			**X**
Climate change		X	X
Human toxicity - cancer			X
Human toxicity – non-cancer			X
Ecotoxicity			X
Particulate matter			X
Ionizing radiation			X
Ozone depletion			X
Eutrophication terrestrial			X
Eutrophication fresh water			X
Eutrophication marine			X
Ozone formation			X
Acidification			x
Fossil resources			X
Mineral and metals resources		X	X
Land use			X
Water use		X	X

Table 22. Overview of relevant life cycle assessment frameworks

Number	URL	Recommended by	Reasons for recommendation	Highlighted features	Description of framework
1	https://www.iso.org/standard/37456.html	Sébastien ARTOUS (CEA)	ISO standards are commonly used for LCA	Environmental management — LCA — Principles and framework	ISO 14040:2006 covers life cycle assessment (LCA) studies and life cycle inventory (LCI) studies.
2	https://www.iso.org/standard/38498.html	Sébastien ARTOUS (CEA)	ISO standards are commonly used for LCA	Environmental management — LCA — Requirements and guidelines	ISO 14044:2006 specifies requirements and provides guidelines for LCA including: definition of the goal and scope of the LCA, the life cycle inventory analysis (LCI) phase.

5.4 Life cycle costing (LCC)

Life-cycle costing is a powerful and indispensable technique used in the construction industry to predict and evaluate the cost performance of assets throughout their entire life cycle. It is a form of analysis that enables clients to determine whether a project meets their performance requirements, taking into account all costs associated with the asset, from acquisition to disposal. Life-cycle costing involves analysing current economic data from clients and the construction industry to assess the costs and benefits of different options. The methodology for life-cycle costing assessment is outlined in the ISO 15686-5 reference document (Table 24), which provides guidance on how to effectively evaluate the costs of constructed assets over their entire life cycle. With life-cycle costing, decision-makers can gain a comprehensive understanding of the financial implications of different choices, including not only initial costs but also ongoing operating costs, maintenance costs, and even disposal costs, along with the time value of money. By considering the full life cycle costs of constructed assets, life-cycle costing empowers organizations to make informed decisions, optimize their investments, and achieve better cost performance while meeting client requirements. Table 23 summarises the information needed to carry out a life cycle cost assessment according to the different levels.

5.4.1 Overview of information needs

Table 23 Life cycle costing (LCC) information needs mapped to the innovation process

Information needs	Early in the innovation process	Mid in the innovation process	Late in the innovation process
Construction costs if applicable (professional fees, temporary works, construction of asset, initial adaptation or refurbishment of asset, taxes, other).	x		
Operation costs if applicable (rent, insurance, cyclical regulatory costs, utilities, taxes, other).		x	
Maintenance costs if applicable (maintenance management, adaptation or refurbishment of asset in use, repairs and replacement of minor components, replacement of major systems and components, cleaning, grounds maintenance, redecoration, taxes, other).		x	
End of life costs if applicable (disposal inspections, disposal, reinstatement to meet contractual requirements, taxes, other).			x
Recycling costs			X

SURPASS

5.4.2 Overview of relevant frameworks

Table 24 Overview of relevant life cycle costing impact assessment frameworks

Number	URL	Recommended by	Reasons for recommendation	Highlighted features	Description of framework
1	https://www.iso.org/standard/61148.html	Daniel Ganszky (GEO)	Such ISO standards are commonly used for both LCA and LCC.	Performance requirements in the context of the project life cycle, taking in account analysis at different stages of life cycle.	ISO 15686-5:2017 provides requirements and guidelines for performing life-cycle cost (LCC) analyses of buildings and constructed assets and their parts, whether new or existing.

LCCA results and hotspots can be visualised in multiple ways including bar plots, line graphs etc. Whichever options helps the reader visualise the differences between the reference and the novel products works best. Using a radar-chart might be the most visually appealing way to show the differences in construction, operation, maintenance, end-of-life cost between the reference and the novel product.

5.5 Social sustainability considerations

Even though the first priority of SURPASS is the safety and environmental impact, social sustainability is also an important component. The methodology to assess social sustainability is a Social-LCA to support sustainable design of products; to support Human Rights Due Diligence of organizations; to identify main social hotspots of a product and/or organization; to quantify and qualify the potential social performance of products and/or related impacts, in order to support sustainable consumption; to examine potential social improvement options along the life cycle; to assess the most relevant stages in the social value chain in terms of social impacts/hotspots (materiality, transparency); to assess and compare, when possible, potential social performance and/or social impacts of product-systems; to communicate the potential social performance and/or social impacts of the product to the public; and to understand if the product value chain contributes to the social development of its stakeholders. A list of possible social parameters to account for was made in Table 25 which was adapted from UNEP [23].

Although the SURPASS project does not plan to deal with the social aspect, it seems interesting to propose here the approach that could be implemented to conduct a social assessment.

In Table 25, some of the social parameters have been put in bold. They were selected from the whole set as those who fit best to the potential social issues raised for the three sectors related to the case studies in tables 5 to 7. Among these preoccupations have been raised "child labour", "accident at work" or "awareness about overconsumption" for example. The selection of social parameters put in bold try to reflect them and provide an insight on these impacts according to the stakeholder that might be affected.

As the S-LCA guidelines provided by the UNEP do not make the link with innovation processes and temporality through a development process, no direct link could be made with the three steps that the project defined (early, mid, late). Nevertheless, we think interesting to propose a temporal perspective on the assessment of these indicators along the innovation process. In the early stages of the process, could be considered the social parameters put in bold in the table above, whose selection follows the first identification of potential issues related to the different sectors concerned. As they seemed to be the most evident for the experts involved in the project, a first evaluation to confirm or infirm this first intuition could be from a great help. Although they could be helpful at the beginning of the process, they do not provide an exhaustive and representative view of the whole potential impacts. As the innovation process evolves and the characteristics of the product systems and the stakeholders that might be affected become more precise, we would recommend to extend the set of social parameters considered. We would also encourage, following the recommendations of the UNEP, to consult the stakeholders to help with the selection.

Table 25. Possible social parameters for future consideration, early, mid and late in the innovation process as social aspects are beyond the work in SURPASS.

Information needs	Early	Mid	Late	Information needs	Early	Mid	Late
WORKERS				*VALUE CHAIN ACTORS (not consumers)*			
Fair salary				**Fair competition**			
Forced labour				Promoting social responsibility			
Health and Safety				Respect of intellectual property rights			
Child labour				**Supplier relationships**			
Freedom of association and collective bargaining				Wealth distribution			
Working hours				*SOCIETY*			
Equal opportunities / discrimination				Corruption			
Skills, knowledge and employability				Prevention and mitigation of armed conflicts			
Social benefits / social security				Technology development			
Smallholders including farmers				Public commitments to sustainability issues			
Management of reorganization				Contribution to economic development			
Employment relationships				Ethical treatment of animals			
Human rights due diligence				Poverty alleviation			
Sexual harassment				Taxation			
Working conditions				*LOCAL COMMUNITY*			
Job satisfaction				Community engagement			
Management of workers individual health				Local employment			
Noise reduction				Safe and healthy living conditions			
Measures to attract women into the workforce or to break down gender segregation in jobs				**Access to material resources (water, minerals, land, biological resources)**			
Pay gap between executives and the average worker not excessive				Respect of indigenous rights			
Implementation of ILO conventions				Access to immaterial resources (e.g. community services, intellectual property			

Information needs	Early	Mid	Late	Information needs	Early	Mid	Late
				rights, freedom of expression, and access to information)			
SMALL SCALE ENTREPRENEURS				Promotion of skills and knowledge			
Meeting basic needs				Secure living conditions			
Access to services and inputs				Inclusion of people with disabilities			
Women's empowerment				Nuisance reduction			
Child labour				Creating and preserving decent jobs			
Health and safety				**Delocalization and migration**			
Land rights				Cultural heritage			
Trading relationships				Access to basic needs for sustainable development			
CONSUMERS				Contribution to economic development			
Health and safety				Access to infrastructure			
Responsible communication				Child care			
Consumer privacy				Promoting community-driven development			
Transparency				Promoting gender equality			
Promotion of skills and knowledge				**Avoiding and addressing negative impacts on communities affected by business operations**			
Consumer product experience				*CHILDREN*			
Accessibility				**Education provided in local community**			
Feedback mechanism				Health issues for children			
Direct impact on basic needs (healthcare, clean water, healthy food, shelter, education)				Children concerns regarding marketing practices			
Impact on vulnerable consumers							
End-of-life responsibility							
Affordability							
Effectiveness and comfort							
Designing products to be durable and repairable							
Ensuring access to quality healthcare							
Improving access to healthy and highly nutritious food							
Improving access to good quality drinking water							
Improving access to good quality housing							
Improving access to education and lifelong learning							

6 Communication and visualization (qualitative scoring)

6.1 Early in the innovation process

A communication and visualization tool will be developed in order to guide SMEs in applying SSbD early in the innovation process. The conceptual development of this tool takes inspiration from the OASIS project ([OASIS (project-oasis.eu)]). The [OASIS model] is a simple and user-friendly screening tool designed to carry out the initial diagnosis, define the improvement plans and evaluate the sustainability and evolution of pilot lines. The incorporation of safety and sustainability requirements in these pilot lines, from the first stages of design and operation of the new processes, constitutes a proactive strategy to ensure equally safe and sustainable future commercial manufacturing processes. Consequently, there is a need to define requirements to guarantee the safety, environmental, social and economic sustainability of these pilot lines, considering at the same time their embryonic and pre-commercial nature. This requires simple safety and sustainability management schemes that are easy to use and apply.

The data in Table 14 and Section 5 is being translated into a dashboard which allows monitoring of the progress of safety and sustainability early in the innovation process by displaying the current and target baselines for the areas of management and results through several radar diagrams for the considered period. There is a main dashboard composed of 1. Functionality, 2. Safety, 3. Environmental Sustainability, 4. Economic Sustainability, and 5. Social Sustainability (Figure 20).

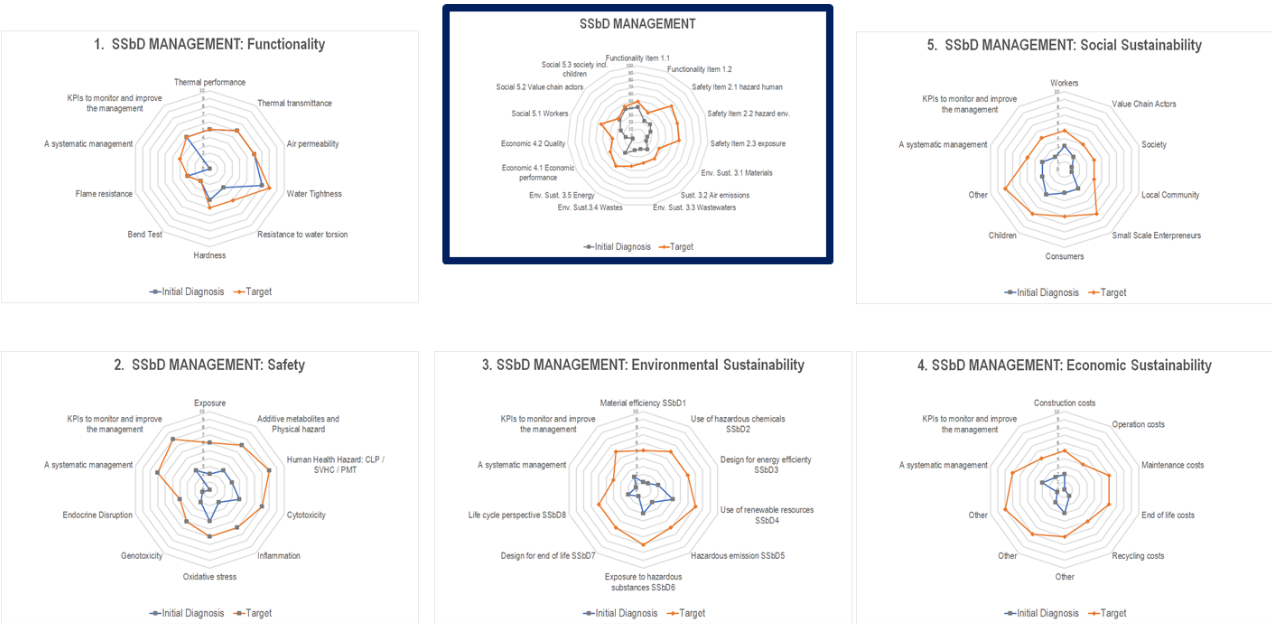

Figure 20. Illustration of the dashboard (SSbD Management) with the different components of 1. Functionality, 2. Safety, 3. Environmental Sustainability, 4. Environmental Sustainability, and 5. Social Sustainability. The components of each dashboard are under development.

Additionally, KPIs for SSbD will be identified to support each of the different components of the dashboard: 1. Functionality, 2. Safety, 3. Environmental Sustainability, 4. Environmental Sustainability, and 5. Social Sustainability (Figure 21).

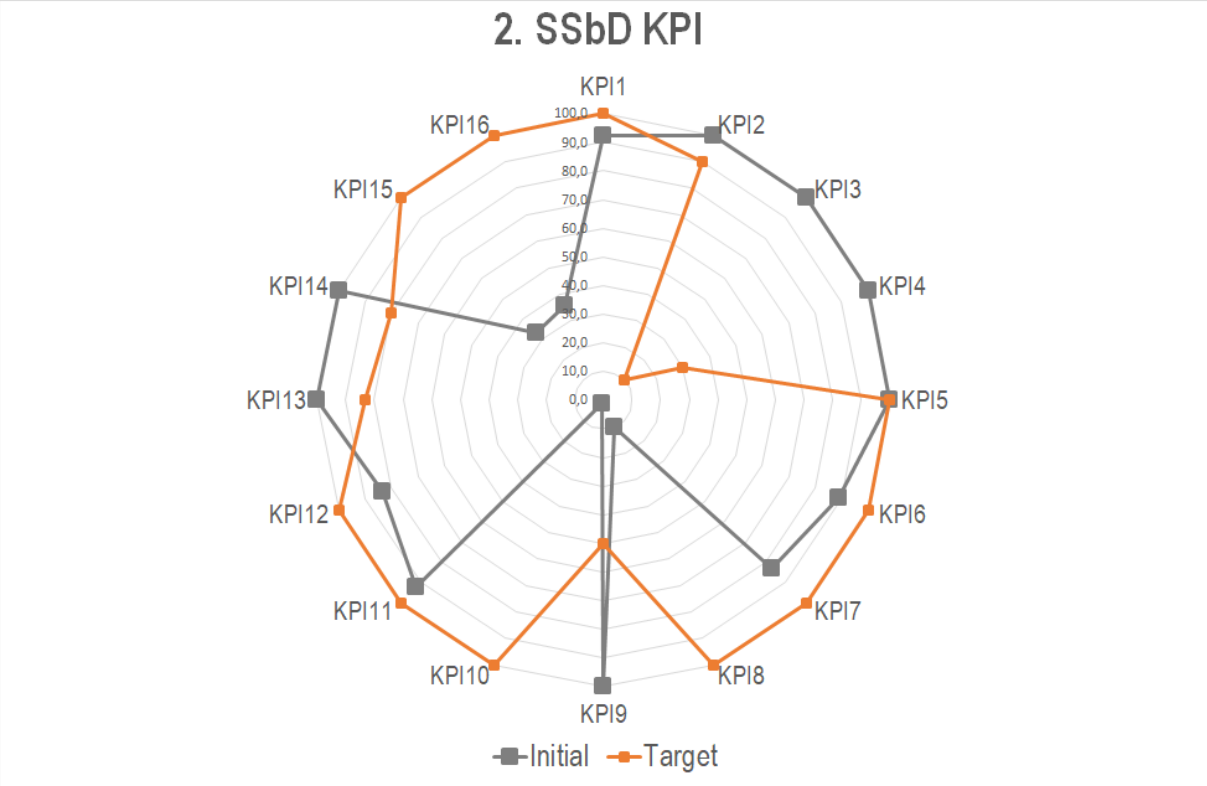

Figure 21. Illustration of KPIs for the monitoring of SSbD management for the different components of 1. Functionality, 2. Safety, 3. Environmental Sustainability, 4. Environmental Sustainability, and 5. Social Sustainability.

6.2 Mid- and Late in the innovation process

For the mid and late stages of the innovation process, the assessment is based on the tables in section 5, which summarise the information needs and the list of indicators. Table 18 refers to Hazard, Table 16 to Exposure, Table 21 to LCA and Table 23 to LCC. At this stage of the innovative process it is not possible to indicate the preferred indicators and the number that will be selected to construct the scoring system. The initial assessment must first be carried out to identify the most relevant indicators for each CS and each pillar of sustainability. Based on these results, the scoring system will be constructed which summarises the information needs and the list of indicators relating to Hazard, Exposure, LCA and LCC.

7 Organizational infrastructure and processes to support SSbD in SURPASS

An interdisciplinary group for case study group encompassing partners from release and exposure (T4.2), Hazard, (T4.3), Health and environmental impact (T4.4) and Life cycle costing (T4.5). Additional teams for social sustainability and qualitative scoring are also developed.

- Release/exposure (task leader Leitat - Camila DELPIVO)
    - CS1 Bastien Pellegrin (CEA)
    - CS2 Camilla Delpivo (LEITAT)
    - CS3 Delphine Tissier (IPC)
    - Patrizia Marie Pfohl (BASF) will focus on microplastic release in all the CS
- Hazard (task leader – RIVM - Yvonne Staal, RIVM)
    - CS1 Ana Candalija (LEITAT)
    - CS2 Thierry Douki (CEA)
    - CS3 Niels Leijten (RIVM)
- LCA (task leader – CEA - Stéphanie Desrousseaux)
    - CS1 Stéphanie Desrousseaux (CEA) and Daniel Ganszky (GEO)
    - CS2 Stéphanie Desrousseaux (CEA) and Daniel Ganszky (GEO)
    - CS3 Sarah Librere (IPC)
- LCC (task leader - GEO - Daniel Ganszky)
    - CS1 Sébastien ARTOUS (CEA)
    - CS2 Daniel Ganszky (GEO)
    - CS3 Mathieu LIONS (IPC)

Figure 22. Organizational infrastructure for the 3 case studies to ensure that each study group consists in partners with expertise in release and exposure (T4.2), Hazard, (T4.3), Health and environmental impact (T4.4) and Life cycle costing (T4.5).

8 Deviations from the workplan

There is no deviation from the workplan

9 Conclusions and perspectives

In this deliverable, a review of previous and on-going SSRbD initiatives was made including monitoring policy developments such as the general framework developed by the EU Commission for framework for SSbD criteria which takes into account the entire life cycle. The operationalization of the SSRbD criteria for polymeric materials was aligned to these ongoing international initiatives and internally with the SURPASS consortia. A series of internal workshops were organized during T4.1 meetings to brainstorm on how to operationalize the proposed SSbD framework from the EC to polymeric material specific SSRbD in a co-creation process involving participants from WP2 & WP3 and risk assessors, toxicologists, hygienists, eco-design and sustainable development experts and regulators. The translation of the EC JRC framework to fit SURPASS project was performed through the development of a holistic life cycle thinking. The Safe-Sustainable-and-Recyclable-by-Design Approach consists of the following steps:

4. The identification of criticality, toxicity, environmental, social, circularity, functionality and economic impacts in a life cycle thinking perspective per case study
5. The development of Safe-Sustainable-and-Recyclable-by-Design strategies
6. Verification of Safe-Sustainable-and-Recyclable-by-Design strategies to ensure they lead to safer and more sustainable alternatives

This first 2 steps are being applied to the 3 cases studies (***Building sector, Case Study CS#1:*** New recyclable-by-design bio-sourced polyurethane (PU) to replace PVC (Polyvinyl Chloride) as insulating material for window frames; ***Transport sector, Case Study CS#2:*** Fire resistant, intrinsically recyclable epoxy-vitrimer materials for sustainable composites to replace metal for train body; ***Packaging sector, Case Study CS#3:*** Recyclable MultiNanoLayered (MNL) films to replace multi-layer films for packaging with drastically reduced concentrations of compatibilizers). These include the identification of criticality, toxicity, environmental, social, circularity, functionality and economic impacts in a life cycle thinking perspective per case study. For each of the case studies, the biggest safety & sustainability challenges, and the development of SSRbD strategies. Ongoing work is on the optimization of the SSRbD strategies and Step 3, which is the verification that these are safer and more sustainable alternatives.

In this deliverable, a communication and visualization (qualitative scoring) dashboard is proposed consisting of 1. Functionality, 2. Safety, 3. Environmental Sustainability, 4. Economical Sustainability, and 5. Social Sustainability. These will be translated to KPIs that can guide SMEs into identifying safety and sustainability hotspots and development of impact-driven SSRbD strategies.

Finally, in terms of internal organization, an interdisciplinary group for case study group encompassing partners from release and exposure (T4.2), Hazard, (T4.3), Health and environmental impact (T4.4) and Life cycle costing (T4.5) was developed and is actively supporting the further development of the SURPASS SSRbD approach.

10 Annex

No Annexes

11 References

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12 Appendices

No Appendices.