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 D1.2

Set of design rules for targeted applications and domains

Work Package	**1**	Landscape analysis for the development of SSRbD polymers and guiding tool
WP Leader		CABRERA Géraldine - IPC
Lead beneficiary		IPC
Contributing beneficiaries		**IPC**, CEA, CID, IND, RIVM
Reviewer		A. Tummino – CEA

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

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	☐

Quality procedure			
Contractual delivery date	31/10/2022		
Actual delivery date	dd/mm/yyyy		
Version accepted by the Steering Board	☒	**Report uploaded via Research Participant Portal**	☐

Acknowledgements

The SURPASS project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement N°101057901. This publication reflects only the author's views and the European Union is not liable for any use that may be made of the information contained therein.

Version history

Version	Date	Partner - Author	Email	Comments[1]
V1.1	16/10/22	IPC-Géraldine Cabrera	geraldine.cabrera@ct-ipc.com	Creation of the template and writing structure
V1.2	25/10/22	IND-Emna Ben Mariem	lab@indresmat.com	Building Case of Study contribution
V1.3	25/10/22	CID-Arrate Huegun	ahuegun@cidetec.es	Transport Case of Study contribution
V2	28/10/22	IPC- Géraldine Cabrera	geraldine.cabrera@ct-ipc.com	Packaging Case of Study contribution and compilation of final report
V2.1	04/11/22	CEA - A. Tummino	andrea.tummino@cea.fr	Proofreading and quality check
V2.2	09/11/22	CEA - S. Clavaguera, S. Artous		Revised version following evaluation
V3	16/11/22	IPC- Géraldine Cabrera		Modifications asked after first revised version

[1] Creation, modification, final version for evaluation, revised version following evaluation, final

Executive summary

The purpose of this deliverable (coordinated by IPC) is the definition of use cases and technical specifications regarding the three application domains of SURPASS: Construction, Transport and Packaging.

For each case study, partners provided the following information:

- **CS#1 Construction (Bio-based PU to replace PVC window frames):** technical data related to feedstock sourcing, quality of conventional materials used in the concerned sector; and additivities (variation related to catalyst systems, flame retardants, foaming agents, stabilizers, etc) will be among the key design parameters to be investigated.
- **CS#2 Transport (Epoxy-composite for the railway sector):** technical requirements to achieve the objective of iso-performance materials, including technical function description, use scenario, testing conditions when relevant on identified gaps (e.g. Shift2Rail Joint Undertaking in the Multi-Annual Action Plan (MAAP) adopted in 2015 for train's composite materials).
- **CS#3 Packaging (Multi-nanolayer films for food packaging):** complementary data related to safety issues (e.g. food contact materials according to ILSI-International Life Sciences Institute) and possibly anticipated additives, either IAS (Intentional Added Substances) or NIAS (Non Intentional Added Substances). Anticipated recycling process and waste streams, as well as identified economic and market requirements.

Particular attention has been paid to the whole life cycle description, impacting the exposure scenario definition. Technical data related to feedstock sourcing, quality of conventional materials used in the concerned sector and additivation (variation related to catalytic systems, flame retardants, foaming agents, stabilizers etc.) are among the key design parameters to be investigated. A first version of a list of legacy additives that need to be removed, modified or substituted will be delivered by WP1 with the support of WP2 and WP3, and will be completed by WP4 through the duration of the Project.

Therefore, the main objective is to support the work of WP4, which is focused on the development and use of SSRbD (Safe and Sustainable by Design) assessment tool, methods, and guidance. Through cross-analysis of this data, partners proposed rules for SSRbD polymers design within the three applications sectors. Such design rules were shared and discussed with others Work Packages partners. Later on, these design rules will be shared with the community through the digital infrastructure, which will be developed in the context of SURPASS Project as well.

<u>Deliverable Review*</u>

	Reviewer #1:			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

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

List of acronyms

EVOH	Ethylene Vinyl Alcohol
FST	Fire, Smoke, Toxicity
IAS	Intentional Added Substances
JRC	Joint Research Centre's
LLDPE	Linear Low Density Polyethylene
MNL	Multi-nano layer
NIAS	Non Intentional Added Substances
OTR	Oxygen Transmission rate
PA	Polyamide
PE	Polyethylene
PE-g-MA	Polyethylene grafted with Maleic anhydride
PU	Polyurethane
PVC	Polyvinyl Chloride
SEM	Scanning Electron Microscopy
SSbD	Safe and Sustainable by Design
SSRbD	Safe, Sustainable, and Recyclable by Design
TEM	Transmission Electron Microscopy
WVTR	Water vapor transmission rate

Table of contents

1 Introduction 8

1.1 Safe-and-Sustainable-by-Design (SSbD) Framework features 10

1.2 Applying SSbD Framework to SURPASS Project 12

2 CASE OF STUDY #1: New recyclable-by-design bio-sourced polyurethane (PU) to replace PVC as insulating material for window frames 13

2.1 Technical specifications 15

2.2 Set of designs rules for target applications and domains 17

3 CASE OF STUDY #2: Fire resistant epoxy-vitrimer materials for sustainable composites for railway sector 19

3.1 Technical specifications 22

3.2 Set of designs rules for target applications and domains 24

4 CASE OF STUDY #3: Recyclable Multi-nanolayered films to replace multi-layer films for food packaging with drastically reduced concentrations of compatibilizers 26

4.1 Technical specifications 31

4.2 Set of designs rules for target applications and domains 33

5 Conclusions and perspectives 36

6 References 38

1 Introduction

Plastic, being predominantly made from fossil feedstock, reached a global annual production of almost 370 Mtons in 2019. Unfortunately, a substantial portion of it is quickly discarded as waste. Almost 70% of the collected plastic waste in the EU (29.1 Mtons) is currently incinerated, landfilled, or exported to other countries causing harm to the economy, wildlife, and eventually to human health. Increasing the recycling percentage is vital to limit global heating to 1.5°C. [1]

Societal urgency dictated by those health and environmental impacts has motivated innovators to develop new solutions to make plastic products safer, more sustainable, and more recyclable by design. However, the lack of targeted guidance, holistic vision, and the existence of multiple definitions, regulations and standards result in ambiguity and multiplication of criteria. [2]

SURPASS aims to overcome this global challenge by developing the first safe-, sustainable-, recyclable-by-design (SSRbD) Assessment and guidance dedicated to polymeric materials. Anticipating beyond material and process, the life cycle of future products, their end-of-life (EoL), and potentially their inclusiveness in the circular economy, SURPASS will provide the indispensable holistic vision. It will bring several disciplines together including material and process scientists, hazard assessment experts, toxicologists, and environmental impact specialists. It will test and further operationalize concepts and criteria, relying on the 3 original pillars of sustainable development: economic, environmental, and social criteria (including safety criteria), and confront them with results from the three sectors representing 70% of the European plastic demand chosen for their industrial relevancy and the need for replacement of non-recyclable materials:

- → ***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.

In particular, WP1 (Landscape analysis for the development of SSRbD polymers and guiding tool) will help building foundation of the main activities scheduled in the project, providing:

- ✓ A deep and dynamic analysis of current policy and regulation landscape
- ✓ Technical specification definition and strict compilation of data related to foreseen benchmark for each case study

- ✓ End-user requirements for the digital infrastructure set up (bottom-up approach to design UI/UX to make it user-friendly.

This deliverable D1.2 is associated with Task 1.2 within WP1, which is focused on the definition of use cases and technical specifications. This task aims to support the developments of materials in WP2 (Development of next generation polymeric materials and additives), of reprocessing technologies in WP3 (Sustainable technologies towards polymer recycling), and the structuration of assessments in WP4 (Development and use of SSRbD assessment tool, methods, and guidance). This task will be mainly managed by the Case Study Leaders: INDRESMAT for CS#1 (bio-based PU to replace PVC), CIDETEC for CS#2 (epoxy-composite for the railway sector), and IPC for CS#3 (Multi-nanolayer films for packaging).

Therefore, for each case study, partners provided the consortium with the corresponding information:

- **CS#1 Construction (Bio-based PU to replace PVC window frames):** technical data related to feedstock sourcing, quality of conventional materials used in the concerned sector, and additives (variations related to catalytic systems, flame retardants, foaming agents, stabilizers, etc.) will be among the key design parameters to be investigated.
- **CS#2 Transport (Epoxy-composite for the railway sector):** design specifications and technical requirements to achieve the objective of iso-performance materials, including technical function description, use scenario, testing conditions when relevant on identified gaps (e.g. Shift2Rail Joint Undertaking in the Multi-Annual Action Plan (MAAP) adopted in 2015 for train's composite materials).
- **CS#3 Packaging (Multi-nanolayer films for food packaging):** complementary data related to safety issues (e.g. food contact materials according to ILSI-International Life Sciences Institute) and possibly anticipated additives, either IAS or NIAS. Anticipated recycling process and waste streams, as well as identified economic and market requirements.

For the three case studies, material sourcing (e.g. bio-based content, recycled material content…), additivation (e.g. covalently bound fire retardants, no compatibilizers …), material processing and reprocessing (e.g. vitrimerization, decontamination …) are among the key design parameters investigated along the project. A first version of the inventory of additives is prepared by WP1 with the support of WP2 and WP3 to describe their properties and function, and will be completed by WP4 with hazard-related data along the duration of the Project.

Since the aim of SURPASS Project is to contribute to the SSRbD (Safe,Sustainable and Recyclable by Design) assessment and guidance dedicated to polymeric materials, particular attention has been paid to the whole life cycle description and the definition of the exposure scenarios, following the SSbD framework.

The safe-by-design (SbD) concept puts emphasis on the identification of the risks and uncertainties concerning human and environmental safety at an early phase of the innovation process in order to minimize uncertainty, exposure and/or hazard(s). In this optic, SURPASS aspires to develop its SSRbD assessment guidance through a product-oriented approach. To implement sustainable-by-design thinking, SURPASS Project will adapt and operationalize the existing documents on SSbD criteria (for chemicals and materials) [3], to fulfill the requirements of SMEs (Small and Medium Enterprise) and be coherent with the current and upcoming regulations.

1.1 Safe-and-Sustainable-by-Design (SSbD) Framework features

The EC JRC (Joint Research Centre's) report proposes a framework outlining the dimensions, aspects, methods, and indicators that can be used to assess chemicals and materials, and how SSbD criteria can be defined in order to identify the materials and chemicals that are SSbD. The framework provides an assessment of the entire life cycle of a chemical or material, including the design phase and considering, among others, its functionality and end-use(s) [4].

The EC JRC recommends a two-phase approach in the report for the SSbD criteria framework:

- ✓ a (re)design phase in which design guiding principles are proposed to support the design of chemicals and materials
- ✓ a safety and sustainability assessment phase in which the safety, environmental and socio- economic sustainability of the chemical/ material is assessed

The safety and sustainability assessment described in the EC JRC allows the identification of SSbD chemicals and materials, and provides a framework where SSbD criteria can later be defined. The overall safety and sustainability assessment comprises five steps:

- → ***Step1:*** Hazard assessment of the chemical/material
- → ***Step2:*** Human health and safety aspects in the chemical/material production and processing phase
- → ***Step3:*** Human health and environmental effects in the final application phase
- → ***Step4:*** Environmental sustainability assessment

→ ***Step 5:*** Social and economic sustainability assessment

These five steps can be carried out sequentially or in parallel, depending on data and tools availability. Moreover, the assessment can be done and, in many cases, should be done iteratively to optimize the results along with redesign of chemicals and materials driven by the results of the different iterative loops.

1.2 Applying 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 1):

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

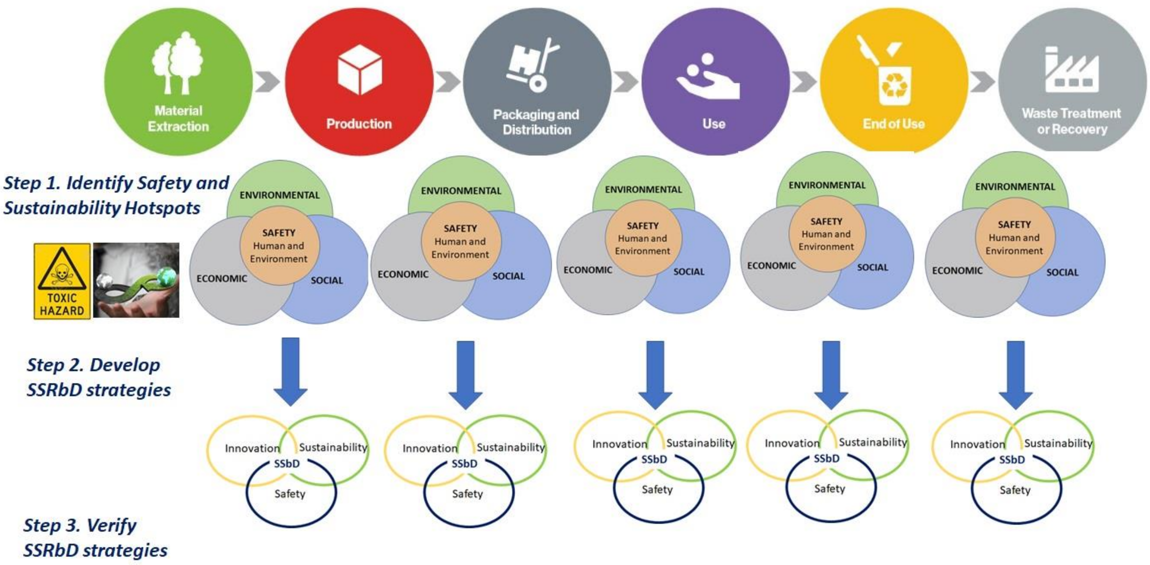

Figure 1 Scheme for the Safe and Sustainable by Design (SSbD) approach applied in SURPASS

The SSbD methodology in Figure 1 was 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 Steps 1 and 2 of the methodology. Step 3 will be performed throughout the project.

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

2 CASE OF STUDY #1: New recyclable-by-design bio-sourced polyurethane (PU) to replace PVC as insulating material for window frames

PU foams are the best and affordable isolation materials present on the market [5]. PU foams have the potential to replace PVC in some building applications, such as the insulating windows frames developed by INDRESMAT.

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.

However, 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).

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.

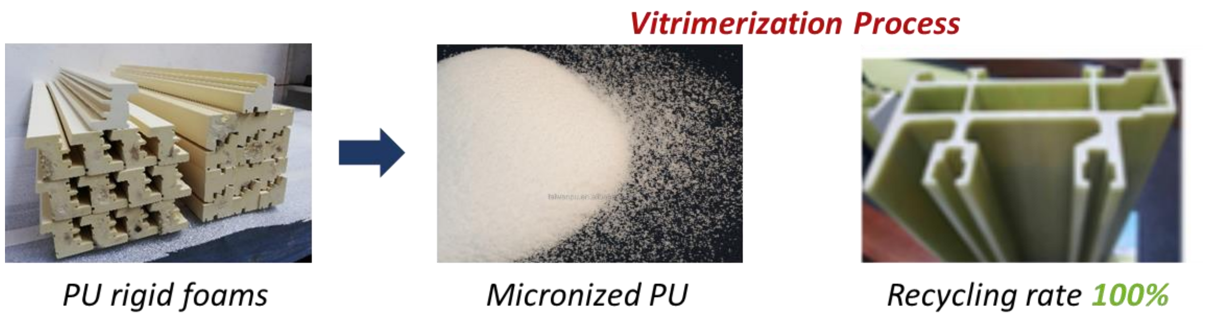

Figure 2 Life stages of PU windows from window frames to 100% recycled material through vitrimerization

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

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.

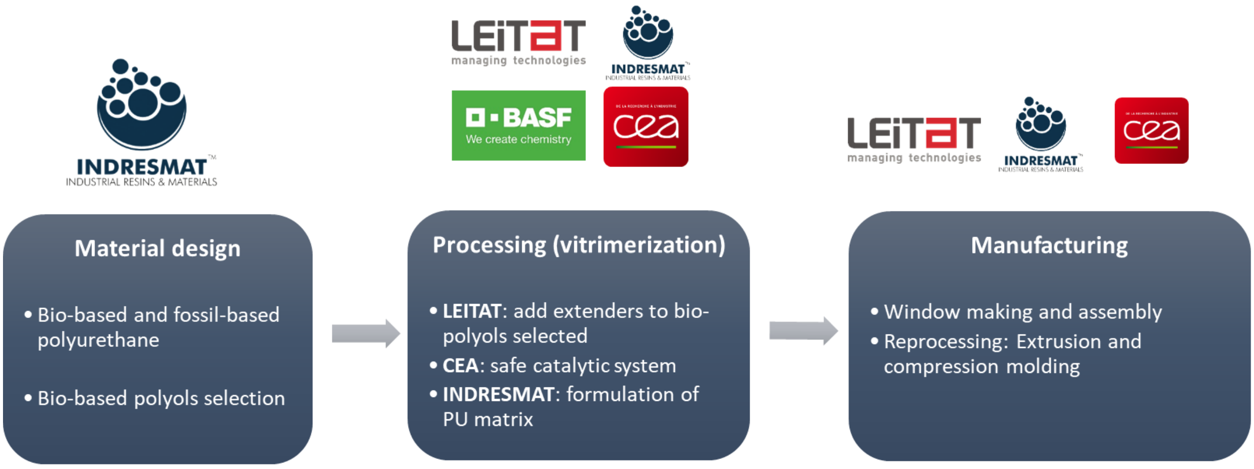

Figure 3 Technical work methodology in case study 1 to obtain recycled and recyclable bio-PU window frames

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.

In the figure below, the comparison between the current product status and the safe and sustainability by design strategies are shown. Going from material design, processing, manufacturing, use and end-of-life to finally reach the SSbD requirements regarding this case study.

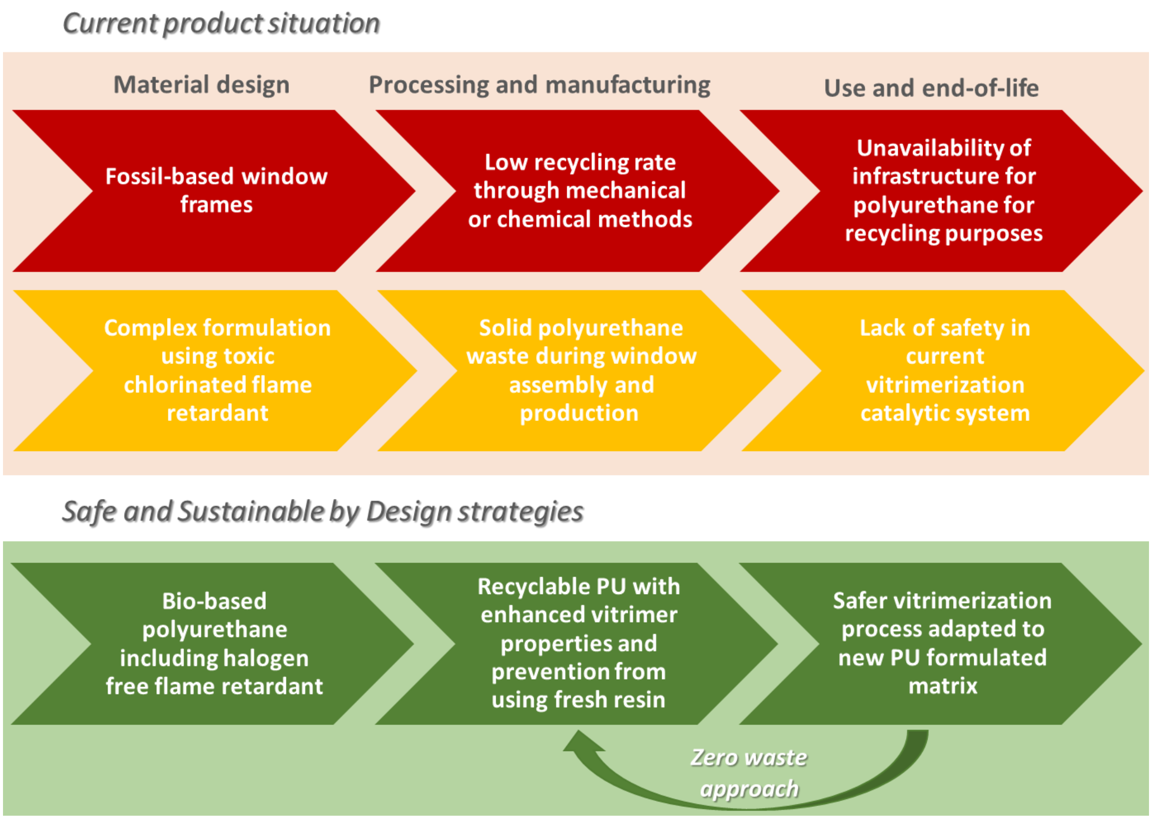

Figure 4 Mapping of the SSbD Approach applied to the Building Case of Study of SURPASS Project

2.1 Technical specifications

INDRESMAT has already introduced fossil-based PU window frame, which have been tested before commercialization. As such, these fossil-based materials serve as a reference for SURPASS. Table 1 contains the results of the tests which evaluated the insulation and mechanical properties of the formulation currently used by INDRESMAT.

The properties of the Bio-sourced PU window frames are expected to be similar (or better) to those that are already commercially available. Although, it is important to mention which compromise can be accepted in case properties are not similar. For instance, properties can be different, but there are major improvements in terms of costs and or safety aspects (human and environmental).

Table 1 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
	Resistance to wind load (EN 12211:2017. Windows and doors. Resistance to wind load)	Global classification: Class C5 Classification standard: EN 12210:2017
Mechanical properties	**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

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

2.2 Set of designs rules for target applications and domains

In this part, we will introduce the SSbD mapping approach developed in the context of SURPASS. Our approach considers the different life cycle stages and their corresponding impacts from the environmental, social, health and safety, and economical perspectives. The following steps are required to implement this approach:

- Table 2: Identification of life cycle stages to be investigated for this Case Study, from raw materials and processing, to the end-of-life of the final product
- Table 3: Evaluate the environmental, social, health and safety, and economic impacts of each life cycle stages

Table 2 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)

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

Table 3 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. -CEA: Integration of catalysts (IAS) in the polymer can increase the production of NIAS + release catalyst, an approach was the catalyst is grafted in the polymer network will be tried to limit this leaching effect -From 2022 there is a restriction in the use of diisocyanates https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:32020R1149	-Solid polyurethane residues (powder, chips) during window assembly -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.	
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	-CEA: 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 but the project target is to replace it by catalysts that are not classified as CMR nor toxic to human or environment	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))	-Integration of catalysts (IAS) in the polymer can increase the production of NIAS + release catalyst - An approach where the catalyst is grafted in the polymer network will be tried to limit this leaching effect. - NIAS identification will be tried to evaluate potential risks for human health/safety	
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. The extrusion step will be done at temperatures as low as possible	Polyurethane products require larger investment from the end user than commodities: raw materials price volatility due to oligopoly nature of polyurethane market	

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

3 CASE OF STUDY #2: Fire resistant epoxy-vitrimer materials for sustainable composites for railway sector

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**.

However, the application of **composite materials** in rolling stock (primary structures) shall 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.

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

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 5.

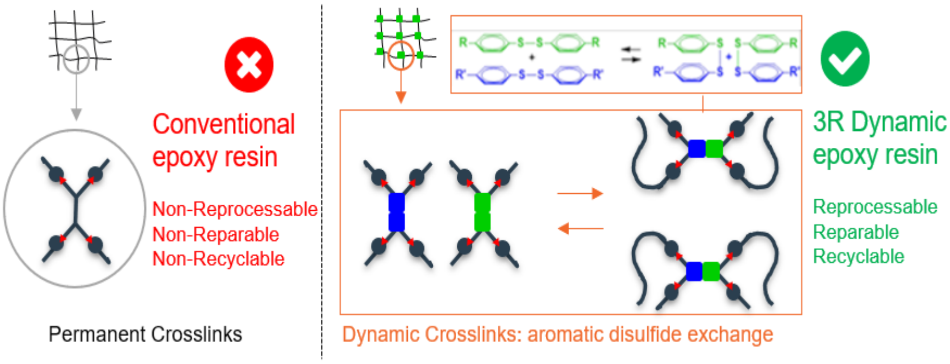

Figure 5 Schematic representation of conventional epoxy vs recyclable 3R epoxy resin

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).

Therefore, to anticipate the growing replacement of metal by non-recyclable composite for structures, **SURPASS Case of Study #2**, targeting the 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.

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.

The roles of the partners involved in developing this approach are well defined and shown in Figure 6, which also schematically depicts the workflow of this case study.

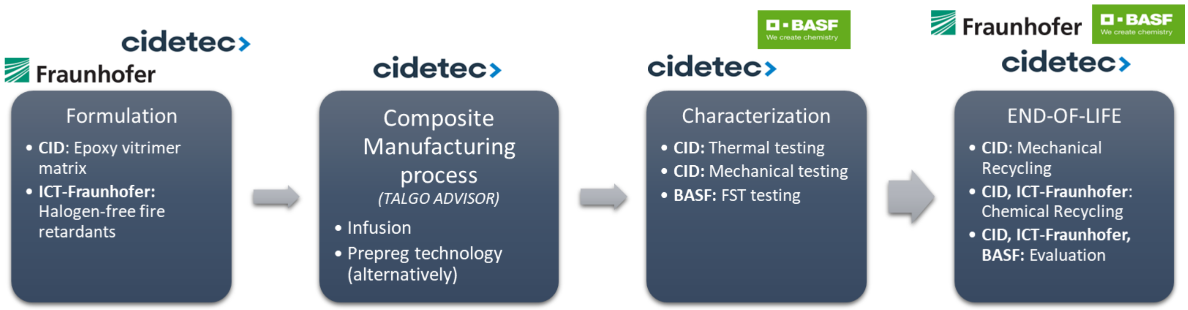

Figure 6 Workflow of the transport case study (railway)

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.

The workflow described in Figure 6 is designed to drive the development of a 3R resin with safer and more sustainable fire retardant properties The mapping (Figure 7) of this case study follows a SSbD strategy that includes the pre-selection of materials, the manufacturing process, the assessment of the entire product life cycle and the post-use (end-of-life) phase.

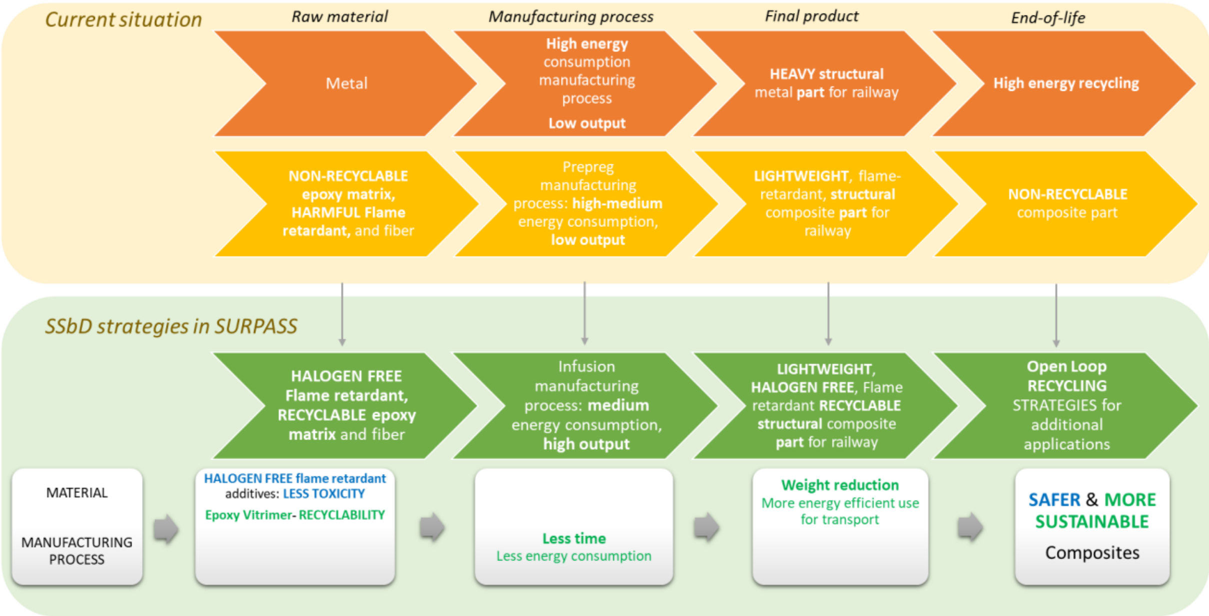

Figure 7 Mapping of the SSbD Approach applied to the Transport Case of Study of SURPASS Project

Figure 7 compares the most relevant differences between currently used raw materials, manufacturing processes and end-of-life strategies. In addition, and as a safer and more sustainable alternative, the SSbD approach of case study 2 is depicted where the most important impacts of each LC stage are indicated, and the objectives and aspirations of SURPASS are discussed.

3.1 Technical specifications

CIDETEC (with the collaboration of ICT and BASF) will work on the formulation of a recyclable epoxy resin.

A table of technical specifications has been prepared (Table 4), where the desired values for mechanical, thermal and fire properties in the context of the SURPASS project objectives are listed.

Table 4 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 527-2
	Tensile Strength at Break (MPa)	> 45	ISO 527-2
	Flexural Strength (MPa)	> 70	ISO 178
Flame resistance (Final Product)	**Hazard level**	HL2[2]	EN 45545-2
	MARHE (kW/m2)	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)*

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

3.2 Set of designs rules for target applications and domains

The mapping of the SSbD approach and the technical specifications describing the key properties for the flame resistant 3R epoxy resin formulations are used to build the life cycle stages analysis and applying the SSbD framework. To build this analysis, the following steps were implemented:

- Identification of the life cycle stages to be evaluated for the case study of Transport, going through raw materials, processing and end-of-life transformation (Table 5).
- Taking each of the selected stages and evaluating their associated impacts in relation to the different aspects of the SSbD approach: environmental, social, health and safety and economic (Table 6).

Table 5 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	

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

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

	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 pollution	**The composite manufacturing** by infusion/RTM required less energy consumption than Prepreg process: Infusion and/or RTM are high throughput processes compared to prepreg technology . For the production of the same number of parts, less energy consumption is required (higher output).	**Mechanical recycling**: the use of waste material to make another material with lower mechanical performance but with properties against fire **Chemical recycling**: use of waste material to recover the reinforcement and cured resin separately so that they can be reused
Social impact	Increased employment to design, build, evaluate and commission an epoxy composites recycling plant through different routes as an alternative to landfill storage of composites or incineration plant activity			
Health-safety impact	Epoxy resin is considered hazardous by OSHA. Causes eye and skin irritation. May cause allergic skin reaction and may also be harmful if absorbed through skin or if swallowed. Di-amine hardener even it is not classified in REACH, its SDS is collected that this material causes skin, eye and respiratory irritation, but it does not meet the persistent, bio accumulative and toxic (PBT) criteria of REACH regulation.	**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 free fire-retardant additives: there are not Brominated fire retardants (toxic)	**Use of Halogen free additives** during processing manufacturing and life cycle: Reduce the health impact of halogenated compounds, particularly on the endocrine system of people exposed to this product (workers and civilians).		
Economic impact	These flame-retardant additives are based on fossil raw materials, which are exhaustible, and many of them are not present in Europe. Flame retardants and hardener are not produced at large scale; therefore, they could be more expensive and insufficient.			

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

4 CASE OF STUDY #3: Recyclable Multi-nanolayered films to replace multi-layer films for food packaging with drastically reduced concentrations of compatibilizers

Nowadays, 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. [11]

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. 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.

In case of Multilayer film's designs like five-layered films, the central layer is often delimited by two adhesive layers that enable adhesion to the outer and inner layers. For example, this structure is common for barrier films with PA or EVOH, since these polymers have poor adhesion to the main structure polymers, copolymers are used as tie-layers in order to compatibilize and improve adhesion between the barrier and the external layers [12]. However, the materials used as compatibilizers can potentially migrate to the product, which represents a great issue for food packaging applications. In addition, the presence of these compatibilizers represents a drawback for the potential reprocessing of these multilayer films, since it can be considered as contaminant to the already existing recycling streams.

SURPASS proposes to evaluate the feasibility to develop Multi-nanolayer (MNL) polymer based films, applying a specific coextrusion technology. In the MNL process, the combination of two or more extruders through a multichannel-layered feedblock is used to produce up to 1000 layers films. Polymer materials separated by different streams are combined into parallel layers in the feedblock

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

before exiting to a film, sheet, or annular die. This effect of nano-structuring allows the processing of multinanocomponent films with good barrier, mechanical and optical properties, theoretically without compatibilizing agents, in order to reduce material costs and improve the recyclability of the final product.

The Multi-nanolayer (MNL) coextrusion is a continuous process which allows in a single step to combine one or several materials in a film composed of up to several thousands of alternating layers in the nanometric range, as described in Figure 8. The tortuosity generated in this way ensure high performances as gas barrier.

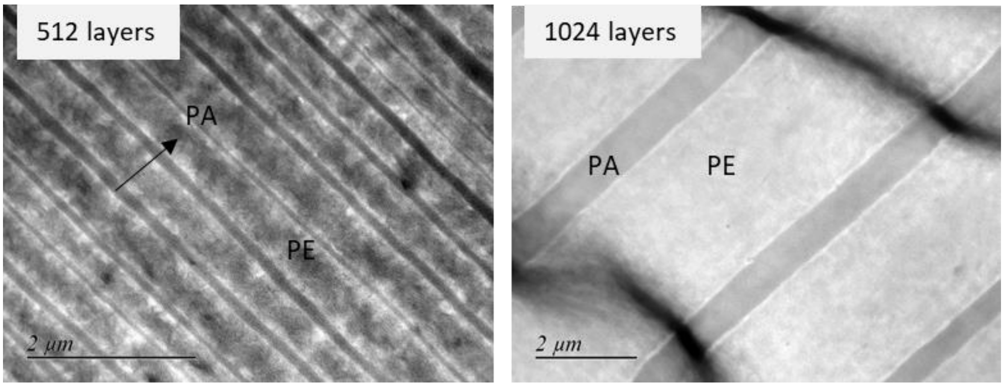

Figure 8 TEM (Transmission Electron Microscopy) images of PE/PA multi-nanolayer film's partial cross section [13]

Films produced by MNL process can theoretically be indefinitely recycled through extensional compounding and reprocessed into a new multilayer film. However extensional compounding can be responsible for degradation of products (because of shear stress, temperature) and release of potentially harmful substances, in particular in view of closed-loop recycling in the food packaging value chain. Therefore, one of the main targets of SURPASS project is to develop the required decontamination process to enable such closed-loop recycling.

Currently, state-of-the art MNL films still contain up to 15% compatibilizers. Hence, SURPASS project aims to develop MNL films containing 0% of compatibilizers.

Cast Forced Assembly Multilayer Coextrusion

Coextrusion is an industrial process commonly used to obtain multilayered sheets or films that can be used for different applications, going from food packaging to microelectronic. These systems can be produced with more than thousands of layers [12] [14]. Coextrusion is a process that combines several polymers via two or three extruders via a feedblock system, where molten polymers from separate extruders are combined together [15]. Each component of the multilayer structure provides their own end-use characteristics. Over time, multilayer polymer-based films with less than 20 layers have been produced in order to improve complex blends film's extrusion process due to performance and cost factors, such as those listed by Ponting et al. [15]:

- Potential reduction in expensive polymer materials by controlling the polymer domain
- Location, continuity, and thickness.
- Incorporation of recycled materials at the internal layers without degrading the film properties.
- Reduce the film thickness maintaining the mechanical, transport, and/or optical film properties.

In SURPASS project, the nanolayer coextrusion processing technique uses a simple two to five layered feedblock with a series of sequential layer multiplication dies. Through the sequential layer multiplication, the two-to-five layered polymer melt flows through a conventional feedblock and then is fed to a series of layer multiplication dies. These layer multiplication dies double the number of layers by a cutting process, spreading and stacking the layered melt stream [12]. As described in Figure 9, the final number of layers in the polymer film is determined as the function of a number of layer multiplication dies, which are placed in series between the feedblock and final film or sheet exit dies. The number of layers of the obtained film can be calculated as a function of the number of layers in the feedblock and the number of layer multiplying dies [16] [17].

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

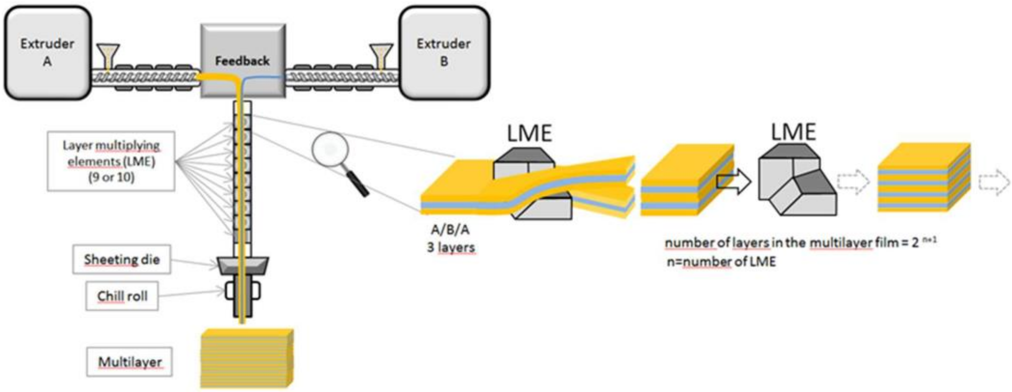

Figure 9 Schematic illustration of layer multiplication in the multilayer coextrusion setup that will be used on SURPASS Project. [18]

Layer multiplication allows structures with hundreds or thousands of layers to be produced. In each multiplier, the initial melt stream is divided vertically into two, spread horizontally, and then recombined, while keeping the total thickness of the melt constant. This allows to double the number of layers and reduce the thickness of each layer after each multiplier. Therefore, the Multi-nanolayer MNL coextrusion is capable of fabricating films having thousands of layers with individual layer thickness down to the nanoscale at low environmental (solvent-free) and budgetary costs [12] [15].

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 (Figure 10), 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. As shown in Figure 10, Polyethylene (PE) will be used as external layers, a copolymer ethylene vinyl alcohol (EVOH) and/or a Polyamide (PA) as the internal layer used as a barrier polymer, and a polyethylene grafted with maleic-anhydride (PE-g-ma) used as a tie-layer in order to improve the adhesion between the internal layer with the external ones.

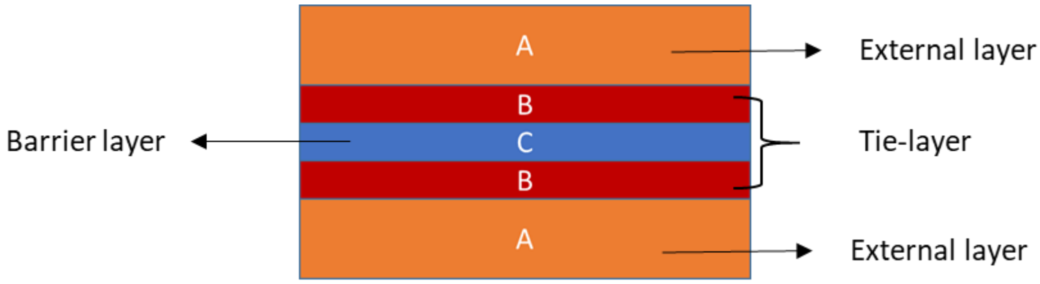

Figure 10 Scheme of the structure of multilayer films containing five layers. Structure chosen as a reference for SURPASS Project, where: A=PE, B=PEgma and C=EVOH and/or PA.

Afterwards, IPC will formulate blends with concentrations of compatibilizers between 0% and 15% applying the multi-nanolayer coextrusion technology, using diverse multiplying elements. The objective is to obtain 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.

The roles of the partners involved in this case of study are well defined and shown in Figure 11. It schematically depicts the workflow of this case study which will be carried out in SURPASS Project.

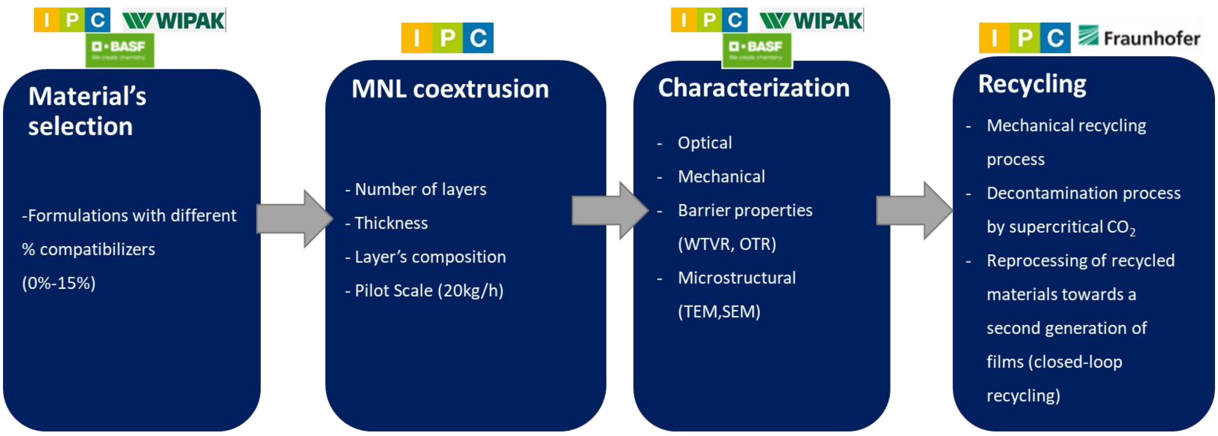

Figure 11 Workflow of the Packaging case of study

To apply the SSbD framework for Case of Study #3 from a holistic point of view, a mapping have been designed (Figure 12). This mapping includes the assessment of the whole life cycle (material sourcing, production, use and end-of life stages are considered). As described in Figure 12, first the whole life cycle assessment of the commercial reference multilayer film will be compared with the targets that SURPASS Project aims to achieve. Therefore, for each particular stage of the multilayer film's life cycle, the implemented SSbD approaches are evaluated, indicating the most important impacts for each of them, and highlighting the SURPASS targets and objectives.

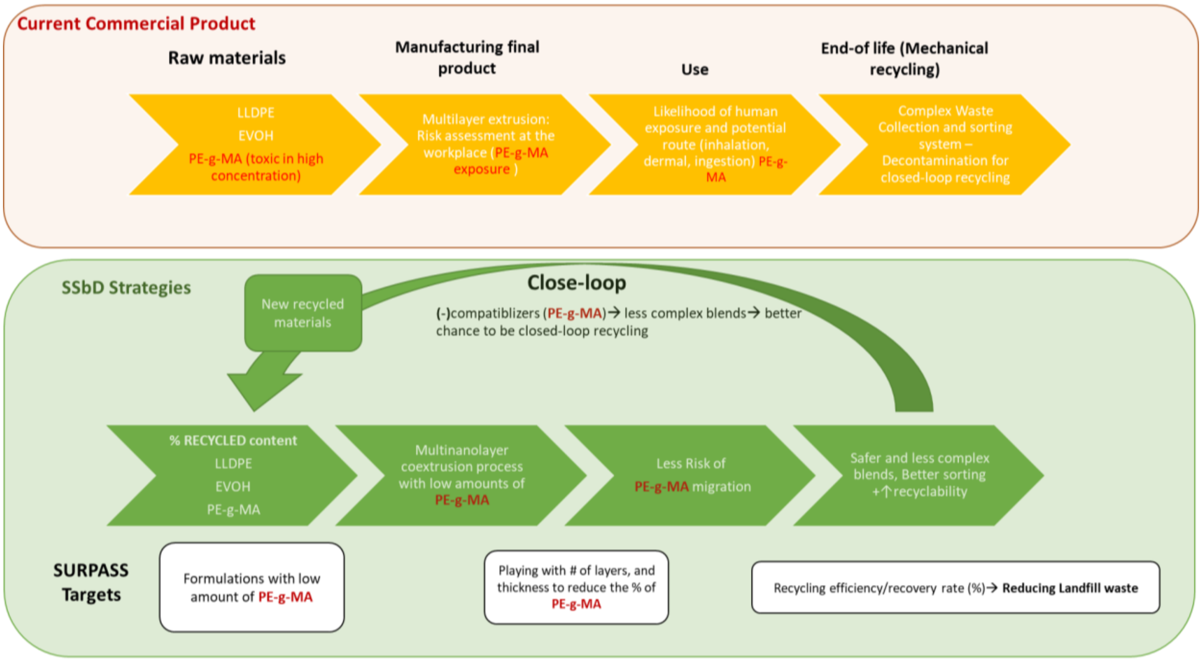

Figure 12 Mapping of the SSbD Approach applied to the Packaging Case of Study of SURPASS Project.

4.1 Technical specifications

IPC (with the support of WIPAK and BASF) will work on the formulation of the reference films, containing up to five layers. Polyethylene (PE) will be used for the external layers, a copolymer ethylene vinyl alcohol (EVOH) and/or a Polyamide (PA) as the internal layer (used as a barrier polymer), and a polyethylene grafted with maleic-anhydride (PE-g-ma) used as a tie-layer in order to improve adhesion between the internal and external layers.

In order to identify the key properties for the formulations of these reference films, a technical specification table (Table 7) has been prepared, highlighting the most important properties in the context of SURPASS project's targets.

Table 7 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/mm^2) 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

4.2 Set of designs rules for target applications and domains

The mapping of the SSbD Approach (Figure 12) and the technical specifications (Table 7) describe the key properties for the formulations of the reference multilayer films, and it served to build the analysis of the life cycle assessment applying the SSbD framework.

In order to build this analysis, the following steps were implemented:

- Identification of life cycle assessments to be evaluated for the Packaging Case of Study, going from the raw materials, processing, to the end-of-life of the final product (Table 8)
- Taking each assessment and evaluate their impact regarding the different aspects of the SSbD approach: Environmental, social, health and safety and economic (Table 9)

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

Table 8 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>Fonction</td><td>External layer</td><td>Barier layer</td><td>Barier 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

Table 9 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 Information for 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 Creation of employment	Creation of employment Assessment of accident at work	Awareness about the overconsumption Pollution in third world countries (export of critical residues) Creation of employment (recycling)	
Health-safety impact	Absence of most harmfull substances according to CSS (EC, 2020) and SVHC of REACH Art. 57 (EU, 2006) Food contact allowed materials	List of chemicals used: apply the ECHA guidance Chapter R12 Use description 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

5 Conclusions and perspectives

The main goal of SURPASS is to contribute developing the first safe-, sustainable-, recyclable-by-design (SSRbD) Assessment and guidance dedicated to polymeric materials. Providing an indispensable holistic vision, it will test and further operationalize concepts and criteria, relying on the 3 original pillars of sustainable development: economic, environmental and social criteria (including safety criteria), by targeting three sectors representing 70% of the European plastic demand: Building, Transport and Packaging.

For this deliverable (D1.2), a life cycle thinking approach was used, impacting exposure scenario definition. The main objective is to support the work of WP4, which is focus on the development and use of SSRbD (Safe and Sustainable by Design) assessment tool, methods, and guidance. Through cross-analysis of these data, partners have proposed rules for SSRbD polymer design for the three applications sectors. These design rules will be shared with others Work Packages and Partners.

In order to fit SURPASS Project, the translation of the EC JRC framework was performed through the development of a holistic life cycle thinking applying the Safe-Sustainable-and-Recyclable-by-Design Approach. This SSbD analysis methodology have been applied to the three case studies of SURPASS, and have been adapted to each application and domain.

This deliverable D1.2 aims to create the framework for the different Work Packages and Partners in SURPASS Project.

It is important to bear in mind that D1.2 is a living document represents only the “starting point” for the investigation. It will serve as a guide for future and that it will be constantly updated during the duration of the Project.

Perspectives

From the set of design rules for targeted applications created for the SURPASS Project, a workflow between the different Work Packages involved has been proposed (Figure 13). This workflow will allow WP2, WP3, and WP4 to work in synergy during the rest of the Project since strategies and roles have been defined. Following and respecting these strategies will be key to the development of the Project.

However, the workflow itself could be refined further to facilitate inter-work package exchanges if needed. Furthermore, 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 co-creation process involving participants from WP2 & WP3, 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), making them applicable to the different plastics investigated in the SURPASS.

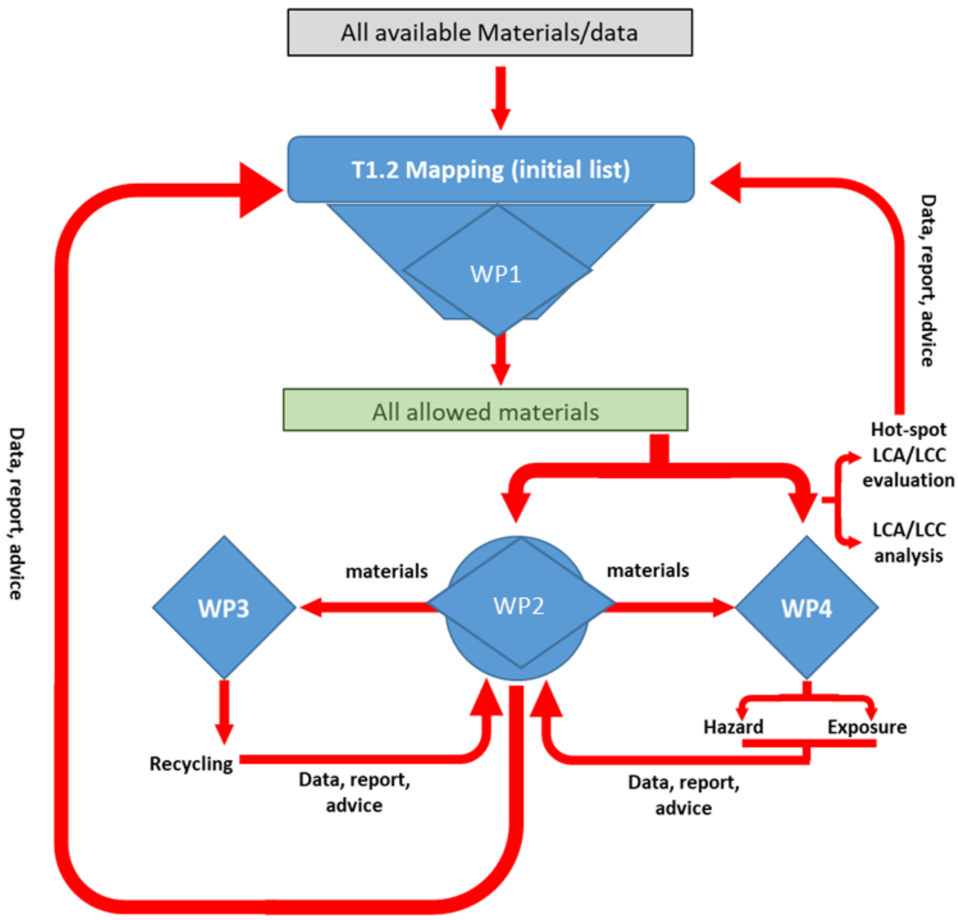

Figure 13 Strategies and workflow created for the future development of SURPASS Project. Sinergy between Work Packages and Partners

Finally, it is also important to mention, that a first version of a list of legacy additives that need to be removed, modified or substituted will be delivered, and will be completed through the duration of the Project.

6 References

[1] Plastics Europe - Association of Plastic Manufacturers, "Plastics – the Facts 2020," *PlasticEurope*, pp. 1–64, 2020, [Online]. Available: https://www.plasticseurope.org/en/resources/market-data.

[2] C. Caldeira, L. Farcal, C. Moretti, L. Mancini, and E. Commission, *Safe and Sustainable chemicals and materials by Design Review of safety and*, no. September 1999. 2022.

[3] OECD, "Moving Towards a Safe(r) Innovation Approach (SIA) for More Sustainable Nanomaterials and Nano-enabled Products. Series on the Safety of Manufactured Nanomaterials.," no. 96, p. No. 96., 2020, [Online]. Available: ENV/JM/MONO(2020)36/REV1.

[4] Caldeira *et al.*, *Safe and Sustainable chemicals by design chemicals and materials*, no. March. 2022.

[5] B. Samali, S. Nemati, P. Sharafi, F. Tahmoorian, and F. Sanati, "Structural Performance of Polyurethane Foam-Filled Building Composite Panels: A State-Of-The-Art," *J. Compos. Sci.*, vol. 3, no. 2, p. 40, Apr. 2019, doi: 10.3390/jcs3020040.

[6] C.-M. Jiao and X.-L. Chen, "Influence of fumed silica on the flame-retardant properties of ethylene vinyl acetate/aluminum hydroxide composites," *J. Appl. Polym. Sci.*, vol. 120, no. 3, pp. 1285–1289, May 2011, doi: 10.1002/app.33126.

[7] L. Chen and Y.-Z. Wang, "A review on flame retardant technology in China. Part I: development of flame retardants," *Polym. Adv. Technol.*, p. n/a-n/a, 2009, doi: 10.1002/pat.1550.

[8] A. B. Morgan and J. W. Gilman, "An overview of flame retardancy of polymeric materials: application, technology, and future directions," *Fire Mater.*, vol. 37, no. 4, pp. 259–279, Jun. 2013, doi: 10.1002/fam.2128.

[9] M. Ciesielski, B. Burk, C. Heinzmann, and M. Döring, "Fire-retardant high-performance epoxy-based materials," in *Novel Fire Retardant Polymers and Composite Materials*, Elsevier, 2017, pp. 3–51.

[10] A. Ruiz de Luzuriaga *et al.*, "Epoxy resin with exchangeable disulfide crosslinks to obtain reprocessable, repairable and recyclable fiber-reinforced thermoset composites," *Mater. Horizons*, vol. 3, no. 3, pp. 241–247, 2016, doi: 10.1039/C6MH00029K.

[11] K. Kaiser, M. Schmid, and M. Schlummer, “Recycling of Polymer-Based Multilayer Packaging: A Review,” *Recycling*, vol. 3, no. 1, p. 1, 2017, doi: 10.3390/recycling3010001.

[12] G. Cabrera, J. Li, A. Maazouz, and K. Lamnawar, “A Journey from Processing to Recycling of Multilayer Waste Films: A Review of Main Challenges and Prospects,” *Polymers (Basel).*, vol. 14, no. 12, 2022, doi: 10.3390/polym14122319.

[13] Q. Lozay *et al.*, “Structural and Barrier Properties of Compatibilized PE/PA6 Multinanolayer Films,” *Membranes (Basel).*, vol. 11, no. 2, p. 75, Jan. 2021, doi: 10.3390/membranes11020075.

[14] B. Lu *et al.*, “Unveiling the Effects of In Situ Layer–Layer Interfacial Reaction in Multilayer Polymer Films via Multilayered Assembly: From Microlayers to Nanolayers,” *Macromol. Mater. Eng.*, vol. 2000076, pp. 1–16, 2020, doi: 10.1002/mame.202000076.

[15] D. Langhe and M. Ponting, “Coextrusion Processing of Multilayered Films,” in *Manufacturing and Novel Applications of Multilayer Polymer Films 1st Edition*, William Andrew, 2016, pp. 16–45.

[16] M. Ponting, T. M. Burt, L. T. J. Korley, J. Andrews, A. Hiltner, and E. Baer, “Gradient Multilayer Films by Forced Assembly Coextrusion,” pp. 12111–12118, 2010.

[17] G. Cabrera, I. Touil, E. Masghouni, A. Maazouz, and K. Lamnawar, “Multi-micro/nanolayer films based on polyolefins: New approaches from eco-design to recycling,” *Polymers (Basel).*, vol. 13, no. 3, pp. 1–21, 2021, doi: 10.3390/polym13030413.

[18] T. Messin *et al.*, “Structure and Barrier Properties of Multinanolayered Biodegradable PLA/PBSA Films: Confinement Effect via Forced Assembly Coextrusion,” *ACS Appl. Mater. Interfaces*, vol. 9, no. 34, pp. 29101–29112, Aug. 2017, doi: 10.1021/acsami.7b08404.