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**Sustainability Assessment along
the life cycle of innovative
materials: the early stage
perspective**

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IndexList

Summary.....	6
List of Contributions	8
Motivations and objectives.....	12
Thesis structure	16
1. Chapter 1 Introduction and Background.....	17
1.1. A transition towards a Safe and Sustainable by-design (SSbD) approach for chemicals and materials	17
1.2. State of the art of the Life Cycle Sustainability Assessment (LCSA)	22
Environmental aspect: Life Cycle Assessment (LCA)	22
Economic aspect: Life Cycle Costing (LCC).....	25
Social aspect: Social Life Cycle Assessment (S-LCA)	26
1.3. SUNSHINE project and case studies.....	27
2. Chapter 2 Methods.....	31
2.1. The SUNSHINE SSbD approach	31
2.2. Tier 1	34
Raw materials and resources needed to produce the material/product.....	39
Production of the MCNM.....	41
Production of the product incorporating the MCNM.....	45
Use of the product	47
End of Life treatment.....	50
2.2.1. Comparison between SUNSHINE SSbD approach and Early4AdMa approach	50
2.3. Tier 2	53
3. Chapter 3 Results	56
3.1. Tier 1 results for anti-sticking coating, active food packaging, and ACRE TFT case studies .	56
3.1.1. Comparison between SUNSHINE SSbD approach and Early4AdMa approach	63
ST1 applied to innovative flame retardant case study	67
ET2 applied to innovative flame retardant case study.....	71
Validation of ST1 and ET2 comparison	73
3.2. Tier 2	75
3.2.1. Anti-stick coating	75
3.2.1.1. Goal and scope definition.....	75

3.2.1.2.	System boundaries	75
3.2.1.3.	Life cycle inventory.....	79
3.2.1.4.	Life Cycle Impact Assessment	84
	LCA	85
	LCC	88
	S-LCA.....	90
3.2.2.	Active food packaging	93
3.2.2.1.	Goal and scope definition.....	93
3.2.2.2.	System boundaries	94
3.2.2.3.	Life cycle inventory.....	96
3.2.2.4.	Life Cycle Impact Assessment	103
	LCA	103
	LCC	106
	S-LCA.....	108
3.2.3.	ACRE TFT	110
3.2.3.1.	Goal and scope definition.....	110
3.2.3.2.	System boundaries	110
3.2.3.3.	Life cycle inventory.....	112
3.2.3.4.	Life Cycle Impact Assessment	114
	LCA	115
4.	Chapter 4 Discussion	120
4.1.	Tier 1	120
4.1.1.	Comparison between SUNSHINE SSbD approach and Early4AdMa approach	125
4.2.	Tier 2	131
5.	Chapter 5 Conclusion.....	137
	Annex 1	151
	Annex 2	152
	Annex 3	155
	Annex 4.....	172

Summary

The European Green Deal, the Chemical Strategy for Sustainability, and the Zero Pollution Action Plan envision a transition towards a toxic-free environment through developing Safe and Sustainable by Design (SSbD) chemicals and materials. To support its implementation, the European Commission (EC) published its Recommendation for establishing a European assessment Framework for SSbD, accompanied by the EC Joint Research Centre's SSbD Framework. Within the context of the Horizon 2020 research programme (H2020) SUNSHINE project, the objective of this thesis was to develop a Safe and Sustainable by Design (SSbD) approach which supports the operationalization of the EC-JRC SSbD Framework. This approach has been designed to be tailored to the needs of companies and society, so that it can support the production and placement on the market of products that not only minimize environmental impacts but also maximize social and economic benefits. The approach enables the assessment of safety and sustainability aspects at each stage of product development from a lifecycle perspective. This is achieved via qualitative (Tier 1) and quantitative (Tier 2) assessment methods. The tiered approach has been applied with different objectives to four case studies in the frame of the SUNSHINE project: (1) a non-stick coating of silica carbide and titanium dioxide for bread baking trays, as an alternative to PFAS-based coatings; (2) a food packaging using nano drops of essential oil on nano clays encapsulated in a polymeric film to keep food insect-free, replacing Low-Density Polyethylene (LDPE); (3) all-carbon recyclable electronic (ACRE) thin film transistors (TFTs) to replace silicon or metal oxide-based semiconductors; (4) a flame retardant made of graphene oxide functionalized with chitosan, substituting melamine cyanuric acid. The results show that Tier 1 significantly supports the early stages of material development by identifying potential safety and sustainability challenges already during R&D when changes to the production process are still feasible and affordable and there is still flexibility in selecting different design options. However, the results also show that if the material or product under analysis is in a very early stage, Tier 1 is difficult to apply because it requires information that may not be known in excessively advanced phases. Tier 2 is instrumental in validating the Tier 1 results and targeting the identified 'hotspots of concern' in more detail later in the innovation process, when more data are available. The tiered approach enables a multi-level evaluation process. When data is scarce, Tier 1 provides an initial qualitative assessment. As more comprehensive data becomes available, Tier 2 allows for

in-depth quantitative analysis. This method ensures early identification and mitigation of potential EHS risks, contributing to the sustainability and efficiency of product development.

List of Contributions

Published paper

Pizzol L., **Livieri A.**, Salieri B., Farcal L., Soeteman-Hernández L. G., Rauscher H., Zabeo A., Blosi M., Costa A. L., Peijnenburg W., Stoycheva S., Hunt N., López-Tendero M. J., Salgado C., Reinosa J. J., Fernández J. F., & Hristozov D., 2023. Screening level approach to support companies in making safe and sustainable by design decisions at the early stages of innovation. *Cleaner Environmental Systems*, 10, 100132. <https://doi.org/10.1016/j.cesys.2023.100132>

Submitted papers

Livieri A., Devecchi S., Pizzol L., Zabeo A., Stoycheva S., López-Tendero M.J., Brunelli A., Badetti E., Semenzin E., Hristozov D. (Submitted to NanoImpact). Assessing Safety and Sustainability Performance of Advanced Nanomaterials: A Tiered Approach to Early Innovation.

Devecchi S., Pizzol L., **Livieri A.**, Zabeo A., Stoycheva S., López-Tendero M., Semenzin E., Brombal D., Hristozov D. (Submitted to Journal of Cleaner Production). Operationalizing Social Life Cycle Assessment for Safe and Sustainable by Design Advanced Materials: the case of multicomponent anti-stick coatings.

Papers in preparation

Livieri A., Pizzol L., Oomen A., Schwirn K., Swart E., Rauscher H., Bleeker E., Gonzalez M., Yamamoto K., Serrano A., Villaro E., Martinez M., Hristozov D. Advancing the development of Safe-and-Sustainable-by-Design toolbox for advanced materials: Complementarities between the SUNSHINE SSbD approach and Early4AdMa.

Livieri A., Doherty J.L., Smith B.N., Franklin A.D., Wiesner M.R., Pizzol L., Hristozov D. Life Cycle Assessment of nano-enabled All-Carbon Recyclable Electronic (ACRE) Materials for Flat-Panel Display.

Book of abstracts

Pizzol L., **Livieri A.**, Salieri B., Soeteman-Hernández L., Hristozov D., 2022. A Safe and Sustainable by Design approach for Multi-component Nano-materials (MCNM). Nano-week & NanoCommons Final Conference. Limassol, Cyprus 20-24 June 2022. Platform

presentation.

Pizzol L., **Livieri A.**, Salieri B., Farcal L., Soeteman-Hernández L. G., Rauscher H., Zabeo A., Blosi M., Costa A. L., Peijnenburg W., Stoycheva S., Hunt N., López-Tendero M. J., Salgado C., Reinosa J. J., Fernández J. F., Hristozov D. 8th International Conference on Health and Safety Issues for a socially responsible approach to nanomaterials. Grenoble (France) 5-9 June 2023. Platform presentation.

Livieri A., Pizzol L., Oomen A., Schwirn K., Swart E., Rauscher H., Gonzalez M., Yamamoto K., Hristozov D. Comparative Analysis between Tier 1 SSbD (Safe and Sustainable by Design) approach and Early4AdMa. SETAC Europe 34th Annual Meeting. Seville, Spain 5-9 May 2024. Platform presentation.

Livieri A., Pizzol L., Devecchi S., Zabeo A., Blosi M., Stoycheva S., López-Tendero M. J., Badetti E., Hristozov D. Life Cycle Sustainability Assessment of nano-enabled PFAS (Polyfluoroalkyl substances)-free anti-sticking coating for bakery moulds. SETAC Europe 34th Annual Meeting. Seville, Spain 5 – 9 May 2024. Poster presentation.

Livieri A., Devecchi S., Pizzol L., Zabeo A., Blosi M., Stoycheva S., López-Tendero M. J., Fernández Lozano J. F., Salgado Soneira C., Brunelli A., Gómez-Cordón J., Villaro Ábalos E., Martinez Junquera M., Serrano Lotina A. M., Bañares M. A., Lloris Cormano J. M., Balbuena J., Saccardo A., Fito C., Barbero Colmenar E., Badetti E., Marcomini A., Semenzin E., Hristozov D. Safe and Sustainable by Design Strategies for the H2020 SUNSHINE case studies. Materials Week 2024. Limassol, Cyprus 17-21 June 2024. Platform presentation.

Livieri A., Doherty J. L., Smith B. N., Franklin A. D., Wiesner M. R., Pizzol L., Hristozov D. Cradle-to-Gate Life Cycle Assessment of Nano-enabled All-Carbon Recyclable Electronic (ACRE) Materials for Flat-panel Displays. Materials Week 2024. Limassol, Cyprus 17-21 June 2024. Poster presentation.

Livieri A., Pizzol L., Oomen A., Schwirn K., Swart E., Rauscher H., Gonzalez M., Yamamoto K., Hristozov D. Advancing the development of Safe-and-Sustainably-by-Design toolboxes for advanced materials: Similarities between the SUNSHINE SSbD approach and Early4AdMa. NanoTox 2024 Venice. 23-25 September 2024. Platform presentation.

Livieri A., Devecchi S., Pizzol L., Zabeo A., Stoycheva S., Semenzin E., Hristozov D. Life Cycle

Sustainability Assessment based Strategy for Safe and Sustainable by Design Advanced Materials. SETAC Europe 26th LCA Symposium. Gothenburg, Sweden 21–23 October 2024. Platform presentation.

Livieri A., Devecchi S., Pizzol L., Zabeo A., Stoycheva S., Semenzin E., Hristozov D. Safe and Sustainable by Design strategies to support advanced nano-enabled material development. SSbD24 Conference Monte Verità. Switzerland 10-15 November 2024. Platform presentation

List of contributions not included in this thesis but related to the thesis research topic

Published papers

Menegaldo, M., **Livieri, A.**, Isigonis, P., Pizzol, L., Tyrolt, A., Zabeo, A., Semenzin, E., & Marcomini, A., 2023. Environmental and economic sustainability in cultural heritage preventive conservation: LCA and LCC of innovative nanotechnology-based products. *Cleaner Environmental Systems*, 9, 100124. <https://doi.org/10.1016/j.cesys.2023.100124>

Stoycheva, S., Peijnenburg, W., Salieri, B., Subramanian, V., Oomen, A. G., Pizzol, L., Blosi, M., Costa, A., Doak, S. H., Stone, V., **Livieri, A.**, Kestens, V., Garmendia, I., Rauscher, H., Hunt, N., Hristozov, D., & Soeteman-Hernández, L. G., 2024. A Conceptual Framework for Safe-and-Sustainable-by-Design to Support Sustainable Business Model Innovation and New Product Development. *Sustainability & Circularity NOW*, 02(CP), a-2498-8902. <https://doi.org/10.1055/a-2498-8902>

Submitted paper

Devecchi S., Pizzol L., **Livieri A.**, Zabeo A., Stoycheva S., López-Tendero M., Semenzin E., Brombal D., Hristozov D. (Submitted to *Journal Cleaner Production*) Operationalizing social life cycle assessment for safe and sustainable by design advanced materials: the case of multicomponent anti-stick coatings.

Book of abstracts

Pizzol L., **Livieri A.**, Zabeo A., Devecchi S., Menegaldo M., Sellitri A., Egizabal Luzuriaga A., Ayerdi Izquierdo A., Oroz T., Ibarrola Moreno O., Hristozov D. Environmental Life cycle assessment applied to medical devices. NANOSAFE 2023. Grenoble, France 5-9 June 2023. Platform presentation.

Pizzol L., **Livieri A.**, Zabeo A., Devecchi S., Menegaldo M., Sellitri A., Egizabal Luzuriaga A., Ayerdi Izquierdo A., Oroz T., Ibarrola Moreno O., Hristozov D. Environmental life cycle assessment applied to medical devices. ICCE 2023. Venice, Italy 11-15 June 2023. Platform presentation.

Motivations and objectives

The European Green Deal aims at transforming the EU's economy to a more sustainable one with policies addressing climate, biodiversity, circularity, human health and environmental protection (European Commission, 2019). This includes an ambitious plan to tackle pollution from all sources and progress towards a zero-pollution economy for a toxic-free environment. The Chemicals Strategy for Sustainability (CSS) and the Zero Pollution Action Plan are driven by the Green Deal ambitions, identify actions to reach them and call for a transition towards a Safe and Sustainable by Design (SSbD) approach for chemicals and materials (European Commission, 2021) (European Commission, 2020). In response to this, the European Commission (EC) published the Recommendation for establishing a European assessment Framework for 'safe and sustainable by design' chemicals and materials (European Commission, 2022). In this thesis, the EC Recommendation (European Commission, 2022) in combination with its scientific-technical background (Caldeira et al., 2022) will be called the "SSbD Framework". The SSbD Framework highlights that assessing health, environmental, social, and economic impacts requires integrated approaches to be able to address complex systems and to enable reproducible and transparent comparison of alternatives to select safer and more sustainable design options (Caldeira et al., 2022). Along with chemical substances, materials and advanced materials (AdMa) fall into the scope of the SSbD Framework. Some categories of multi-component nanomaterials (MCNMs) can be considered Advanced Materials according to the OECD's description of the term (OECD, 2023). The term MCNM itself is not yet well established, neither in a scientific nor in a regulatory context. MCNM may be described as materials that consist of two or more functional components (e.g., nanoparticles, organic molecules) conjugated by strong molecular bonds, or formed by a nanomaterial (NM) with a unique chemical origin modified by hard or soft coatings (Banin et al., 2014; Saleh et al., 2015a); MCNMs can offer significant technological benefits as the integration of different components in a unique system can produce new or improved functionalities. However, MCNMs can also pose substantial design challenges as well as environmental, health and safety (EHS) concerns (Furxhi et al., 2022). The latter are particularly complex due to the differing rates of degradation and different toxicity of the separate and interacting components, and their more complex interactions with biological and environmental systems (Banin et al., 2014; Huang et al., 2018; Saleh et al., 2015b). These concerns

have raised questions regarding not only the EHS implications of these materials, but also their overall sustainability (Mech et al., 2022). The European H2020 SUNSHINE project (h2020sunshine.eu) aimed to address these challenges by developing a comprehensive Safe and Sustainable by Design (SSbD) approach for multi-component nanomaterials (MCNMs) and demonstrating its effectiveness through industrially relevant case studies. This PhD research focused on advancing the SSbD Framework within the SUNSHINE project to enhance the safety and sustainability assessment of MCNMs. As previously mentioned, the SSbD Framework proposed by the European Commission is iterative and follows a tiered approach (European Commission., 2024).

One of the objectives of this thesis was to operationalize the SSbD Framework by developing a tiered assessment approach to evaluate safety and sustainability at different stages of MCNMs development considering various R&D phases, chemical/material maturity and data availability. To achieve this, a first Tier was required for situations where only qualitative information was available, and a second Tier was necessary for cases involving quantitative information. The first Tier was necessary to provide a qualitative assessment tool, such as a questionnaire-based method for the identification of hot-spots and data gaps, for the prioritization of alternatives that presented higher safety and sustainability performance and for the identification of those to be stopped for further development since they presented clear safety and sustainability concerns. This preliminary evaluation is crucial for quickly identifying issues and making informed comparisons. A second Tier was needed to offer a quantitative assessment using Life Cycle Sustainability Assessment (LCSA) methodologies. This more detailed and rigorous analysis quantifies sustainability across the entire life cycle of MCNMs, providing a comprehensive evaluation. Once the tiered approach was developed, there was a need to test its capabilities by applying it to real case studies in the frame of the project in which its development was planned, SUNSHINE. The first case study is a MCNM coating made of silica carbide and titanium dioxide (SiC@TiO₂), which offers non-stick properties for applications such as bread baking trays to be used as an alternative to PFAS-based non-stick coatings, like Teflon®. The second is made of nano drops of essential oil anchored to the surface of nano clays and encapsulated in a polymeric film used as food packaging to keep the packaged food free of insect pests to be used as an alternative for Low-Density Polyethylene (LDPE) The third case consists of an

all-carbon recyclable electronic (ACRE) thin film transistors (TFT) to replace silicon- or metal oxide-based semiconductor materials.

The need for simplified methods that can be applied during the early stage of product development to identify safety and sustainability concerns related to advanced materials has attracted the attention of various research groups across Europe. In parallel with the developments within Sunshine, the Organisation for Economic Co-operation and Development (OECD) proposed the Early Awareness and Action System for Advanced Materials (Early4AdMa) to assist policymakers and regulators in anticipating emerging challenges from AdMA, thereby supporting regulatory preparedness. The Early4AdMa approach also consists of two tiers, both qualitative. Tier 1 involves a screening assessment to identify potential 'concerns', while Tier 2 consists of a more detailed assessment for environmental and human safety, sustainability, and regulatory issues. SUNSHINE Tier 1 and Early4AdMa Tier 2 are both composed of questionnaires for the preliminary analysis of safety and sustainability. Therefore, the last objective of this thesis was to identify similarities, possible overlaps, complementarities between the two approaches, and potential synergies for application by different stakeholders via a comparative analysis. Then, to verify the outcomes of the comparison, it was deemed necessary to test both the approaches on a SUNSHINE case study, an innovative flame retardant made of graphene oxide functionalized with chitosan to substitute classic flame retardant such as melamine cyanuric acid. In this way, the comparison results could assist decision-makers from industry, policy, and regulation in selecting the most suitable methodology for their specific needs. The Tier 1 developed within the context of the SUNSHINE project will be referred to as "SUNSHINE Tier 1" when comparing it to Early4AdMa Tier 2, to avoid any confusion for the reader.

Scope of thesis

The tiered approach developed in this thesis is structured into Tier 1 and Tier 2. Tier 1 consists of a questionnaire designed for the pre-evaluation of safety, sustainability, and functionality. This qualitative assessment helps guide the selection of the most promising design alternatives to develop safer and more sustainable materials and products. Although sustainability is the core focus of this thesis, safety remains an essential aspect of Tier 1, as it was developed in collaboration with experts and is well integrated into both the evaluation process and the way results are presented. For this reason, safety has been retained as part of the thesis.

In contrast, Tier 2 incorporates the REACH Chemical Safety Assessment (CSA) approach and Life Cycle Sustainability Assessment (LCSA) methodologies. Since safety is assessed separately at this stage, it does not fall within the scope of this thesis. Instead, the focus is placed on Steps 4 and 5 of the EC-JRC framework, which encompass Life Cycle Assessment (LCA), Life Cycle Costing (LCC), and Social Life Cycle Assessment (S-LCA), ensuring a thorough and holistic sustainability evaluation.

Thesis structure

According to the objectives outlined above, the thesis was structured as follows.

Chapter 1 Introduction and Background covers the transition towards a safe and sustainable by design (SSbD) approach for chemicals and materials over the years. It also provides an overview of the current state of the art of Life Cycle Sustainability Assessment (LCSA) and describes the project in which the SSbD approach was developed, along with the case studies to which it was applied.

Chapter 2 Methods describes the process for the development of the tiered approach. Also, it presents the methodology used to compare the first tier developed within SUNSHINE and Early4AdMa Tier 2.

Chapter 3 Results reports the outcomes of the application of the tiered approach to different case studies, along with those of the comparison between the first tier developed within SUNSHINE and Early4AdMa Tier 2.

Chapter 4 Discussion examines the results obtained from the application of the tiered approach to different case studies and those obtained from the comparison between the first tier developed within SUNSHINE and Early4AdMa Tier 2.

Chapter 5 Conclusion includes considerations on the main findings of the developed activities, pointing out research limitations and potential future developments.

1. Chapter 1 Introduction and Background

This chapter overviews the transition towards the Safe and Sustainable by Design (SSbD) approach for chemicals and materials over the years. It presents a brief state-of-the-art review of Life Cycle Sustainability Assessment (LCSA) methodologies and introduces the project where the SSbD approach, the focus of this study, was developed, along with the case study to which it has been applied.

1.1. A transition towards a Safe and Sustainable by-design (SSbD) approach for chemicals and materials

As already anticipated in the “Motivation and objectives” section, the European Green Deal aims to transform the EU's economy into a more sustainable one with policies addressing climate, biodiversity, circularity, human health and environmental protection (European Commission, 2019). This includes an ambitious plan to tackle pollution from all sources and progress towards a zero-pollution economy for a toxic-free environment. The Chemicals Strategy for Sustainability (CSS) and the Zero Pollution Action Plan are driven by the Green Deal ambitions, identify actions to reach them and call for a transition towards a Safe and Sustainable by Design (SSbD) approach for chemicals and emerging advanced materials (European Commission, 2021) (European Commission, 2020). In response to this, the European Commission (EC) published the Recommendation for establishing a European assessment Framework for ‘safe and sustainable by design’ chemicals and materials (European Commission, 2022), which is based on a holistic scientific-technical approach developed by the EC's Joint Research Centre (Caldeira et al., 2022). In the following parts of the thesis, the EC Recommendation (European Commission, 2022) in combination with its scientific-technical background (Caldeira et al., 2022) will be called the “SSbD Framework”. The SSbD Framework highlights that assessing health, environmental, social, and economic impacts requires integrated approaches to be able to address complex systems and to enable reproducible and transparent comparison of alternatives to select safer and more sustainable design options (Caldeira et al., 2022). Also, the SSbD Framework foresees the 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) (Caldeira et al., 2022).

The SSbD Framework is designed to establish criteria for SSbD chemicals and materials. The methodology for criteria definition is based on the hazard classes and categories established within the CLP regulation (Regulation (EC) No 1272/2008) as well as REACH (Regulation (EC) No 1907/2006)(Caldeira et al., 2022). REACH, established under Regulation (EC) No 1907/2006, requires manufacturers and importers to gather information on the properties of chemical substances and assess their potential risks. This information is documented in a Chemical Safety Report (CSR), which includes critical components such as hazard assessments, exposure scenarios, and risk management measures. Hazard assessments focus on identifying the intrinsic properties of a chemical that may pose risks to human health or the environment, including toxicity, flammability, and ecotoxicity. These assessments are essential to evaluate the chemical's potential dangers at its source. Exposure Scenarios describe how a chemical substance is used and the resulting likelihood of human or environmental exposure. These scenarios consider factors such as concentration, duration of exposure, and the environments in which the substance is handled. Finally, Risk Management Measures are strategies implemented to minimize or eliminate the identified risks. These can include engineering controls, personal protective equipment (PPE), or restrictions on usage to ensure safety across the chemical's lifecycle. CLP, governed by Regulation (EC) No 1272/2008, complements REACH by standardizing the classification, labelling, and packaging of chemicals and mixtures. It adopts the Globally Harmonized System (GHS) to ensure consistency in hazard communication across the EU. Through clear hazard pictograms, signal words, and precautionary statements, CLP enables users to understand and manage chemical risks effectively. It is based on fundamental principles derived from expert consultations and feedback from stakeholders. As mentioned above, the methodology for criteria definition within the SSbD framework is based on the hazard classes and categories established within the CLP and REACH regulation. Indeed, one of the objectives of the SSbD Framework includes replacing or reducing the use of hazardous substances and minimizing climate and environmental impacts throughout the chemical/material lifecycle while maintaining functionality. The framework adopts a hierarchical approach that prioritizes safety considerations, followed by environmental, social, and economic aspects. It consists of a (re)design phase, where guiding principles support the design of chemicals and materials, and an assessment phase, which

evaluates their safety, environmental impact, and socio-economic sustainability. The safety and sustainability assessment are organized into five steps:

1. Hazard assessment of the chemical/material: Assessing the inherent hazard characteristics of the chemical or material.
2. Human health and safety aspects in the chemical/material production and processing phase: Evaluating potential health impacts during production and processing stages.
3. Human health and environmental aspects in the final application phase: Examining health and environmental effects during the application phase.
4. Environmental sustainability assessment: Assessing environmental impacts across the entire lifecycle.
5. Scientific basis for the socio-economic sustainability assessment: Investigating socio-economic dimensions to be further developed in the future.

According to the EC Recommendation (European Commission, 2020), the proposed Framework is based on a tiered approach depending on data availability, considering that the information available for newly developed chemicals or materials could be limited at the beginning of the process, while it increases along the product development process. Methods and standards are available to assess safety and sustainability during the later phases of product development. However, simplified methods which can be applied in the early stage of product development are still lacking or in the initial stage of development. Specifically, in the initial product R&D phases, where quantitative information on the material/product manufacturing, use and end of life can be patchy or even missing, there is a need for qualitative, screening approaches which are able to identify potential safety and sustainability issues at an early R&D phase. Screening approaches can also reveal information gaps and raise awareness of potential safety and sustainability concerns, which may in turn trigger the need for regulatory action.

Several Frameworks exist that aim to combine safety and environmental, economic, and social assessment from a sustainable development perspective. Examples of Frameworks primarily focusing on chemicals and not specifically addressing nanomaterials and MCNMs include the work developed by the company Evonik (Evonik, 2020), by the Interstate Chemicals Clearinghouse (IC2,

2017), the Alternatives Assessment Framework proposed by Rossi and colleagues (Rossi et al., 2006), the work developed by the UB (Umweltbundesamt (Hrsg.), 2016), and that by the WBCSD (World Business Council for Sustainable Development) (WBCSD, 2018). Additionally, some Frameworks do focus on nanomaterials, such as the LICARA nanoscan (Van Harmelen et al., 2016) which covers public health and environmental risks, occupational and consumer health risks, but also environmental, economic and societal benefits. Additionally, the "Precautionary Matrix" (Höck et al., 2013) is a useful tool for identifying possible risks in the development, production, use, and disposal of synthetic nanomaterials. However, it places less emphasis on sustainability. On the other hand, ReCiPe (Goedkoop et al., 2008) specifically addresses sustainability aspects, but primarily in a quantitative manner.

To facilitate the qualitative assessment of aspects such as safety, environmental, economic, and social sustainability, as well as functionality, several questionnaires have been developed. Among these, the work of (Giese et al., 2020) presents a 20-question framework to assess advanced materials that addresses dimensions like safety, environmental sustainability, economic sustainability, functionality, and regulation. In comparison, the work by (Wiek et al., 2007) to assess emerging technologies presents a more extensive questionnaire with 36 questions, exploring areas such as safety, environmental, social, and economic sustainability, regulation, and a more detailed consideration of functionality. The Early4AdMa framework to address advanced materials includes 65 questions, covering aspects of safety, environmental sustainability, and regulation with a high level of detail (OECD, 2023). Additionally, the above mentioned LICARA nanoSCAN, focuses on nanoproducts, involves 57 questions and provides a comprehensive assessment of safety, environmental, social, and economic sustainability, as well as regulation (Van Harmelen et al., 2016). These questionnaires address a wide range of aspects, but they have a relatively limited number of questions. As a result, while they do cover the identified dimensions—such as safety, environmental, economic, and social sustainability—they tend to do so without delving into a high level of detail. This limitation may affect their ability to capture nuanced insights for more comprehensive evaluations.

For an assessment at a higher tier, where more information is available, SSbD approaches are already available in literature. These have been applied to assess the sustainability of indigo dyeing color in

the fashion sector (Lai & Chang, 2021) or of inhibitors in pharmaceutical products (Romeiro et al., 2019), the design of cellulosic bioelectricity supply chain networks (Yue et al., 2014), the design of a commercial building in Shanghai (Wang et al., 2010) and the sustainability of mechatronic systems application to a regenerative braking system (Mehdi & Boudi, 2021).

As far as the definition of SSbD is concerned, the CSS describes it as: “a pre-market approach to chemicals design 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. In this context, the overall sustainability should be ensured by minimising the environmental footprint of chemicals in particular on climate change, resource use, ecosystems and biodiversity from a life cycle perspective”(European Commission, 2020). Also, “the SSbD approach addresses the safety and sustainability of the material/chemical/product and associated processes along the whole life cycle, including all the steps of the research and development (R&D) phase, production, use, recycling and disposal” (OECD, 2022).

Along with chemical substances, materials and advanced materials (AdMa) fall into the scope of the SSbD Framework. Some categories of multi-component nanomaterials (MCNMs) can be considered Advanced Materials according to the OECD’s description of the term (OECD, 2023). These materials are often referred to as being among those Key Enabling Technologies (KETs) that could support the transition towards more sustainable innovation in key industrial sectors such as construction, structural and functional materials, active ingredients, food, healthcare, energy, cosmetics and electronics (Gottardo et al., 2021; Samani et al., 2015; Zheng et al., 2021). The term MCNM itself is not yet well established, neither in a scientific nor in a regulatory context. MCNM may be described as materials that consist of two or more functional components (e.g., nanoparticles, organic molecules, etc.) conjugated by strong molecular bonds, or formed by a nanomaterial (NM) with a unique chemical origin modified by hard or soft coatings (Banin et al., 2014); (Saleh et al., 2015b). Some of the most widely used components are (combinations of) carbonaceous (e.g., fullerenes, carbon nanotubes, graphene) or metallic (metal or metal oxide) NMs with or without organic coatings (e.g., polymers, macromolecules and enzymes).

MCNMs can offer significant technological benefits as the integration of different components in a unique system can produce new or improved functionalities. However, MCNMs can also pose substantial design challenges as well as environmental, health and safety (EHS) concerns (Furxhi et al., 2022). The latter are particularly complex due to the differing rates of degradation and different toxicity of the separate and interacting components, and their more complex interactions with biological and environmental systems (Banin et al., 2014; Huang et al., 2018; Saleh et al., 2015b). These concerns have raised questions regarding not only the EHS implications of these materials, but also their overall sustainability (Mech et al., 2022). The EU Commission has funded several research projects to address these questions, including HARMLESS (GA 953183), DIAGONAL (GA 953152), and SUNSHINE (GA 952924).

The European H2020 SUNSHINE project (h2020sunshine.eu) strives to provide answers to some of these questions. Its goal was to develop an overarching approach for SSbD of MCNMs and demonstrate it in industrially relevant case studies.

Given the specific characteristics of the SSbD Framework, which is designed to be applied throughout the entire life cycle of chemicals and materials and considering the growing importance of Life Cycle Sustainability Assessment (LCSA) in this context, the state of the art regarding LCSA methodologies is discussed in the next chapter.

1.2.State of the art of the Life Cycle Sustainability Assessment (LCSA)

Life Cycle Sustainability Assessment (LCSA) is a widely recognized measurement tool used to standardize and quantify the impacts of any service, industrial system, or manufacturing process across environmental, economic, and social aspects (R. Lin et al., 2020b). LCSA encompasses three individual methodologies: Life Cycle Assessment (LCA) for environmental analysis, Life Cycle Costing (LCC) for economic analysis, and Social Life Cycle Assessment (SLCA) for social analysis (R. Lin et al., 2020a). In the next paragraphs, these three methodologies are presented.

Environmental aspect: Life Cycle Assessment (LCA)

LCA is a standardized scientific method for systematic analysis of flows (e.g., mass and energy) associated with the life cycle of a specified product, a technology, a service or a manufacturing

process (ISO 14040, 2021). LCA involves quantifying how material and energy flows, documented during the inventory phase, contribute to a series of environmental impact categories, referred to as midpoint categories. These categories cover critical environmental aspects such as climate change, eutrophication, acidification, and resource depletion. This method is employed across diverse industrial and research sectors to evaluate environmental impacts such as Global Warming Potential, Acidification potential, Water use and Scarcity, throughout a product's entire life cycle. LCA enables the assessment of impacts from raw material extraction, production, use, and end-of-life disposal, introducing the concept of cradle-to-grave assessment (Keiser et al., 2023). Also, LCA provides a Framework to evaluate the interactions between a product's environmental impact and its effects on Human Health, Resource Depletion, and Ecosystem Quality, referred to as Endpoint categories. The methodological foundations for conducting these assessments were established in the 1990s and standardized according to ISO 14040-14044 norms (Vauche et al., 2024). There are several approaches to LCA, and each approach offers a unique perspective on environmental impact and can be chosen based on the specific goals of the analysis or the information available at the time of the study. Every approach allows for specific analysis of different stages in a product's life cycle:

1. Cradle-to-Grave: This method involves a comprehensive assessment of the entire life cycle, from resource extraction (cradle) to disposal (grave), covering all stages, including production, use, and disposal phases. This provides a detailed overview of overall impacts.
2. Cradle-to-Gate: The analysis is limited to the phase from resource extraction to the factory gate, excluding the product use and disposal stages. This approach is often chosen when information regarding use and disposal is insufficient.
3. Cradle-to-Cradle: A variant of cradle-to-grave, where the end-of-life disposal phase is replaced by a recycling process. The goal is to minimize environmental impact through sustainable production, use, and disposal systems, promoting social and environmental responsibility.
4. Gate-to-Gate: This approach analyzes only the stages within a single process in the production chain. Results obtained from this method can be integrated to form a more comprehensive assessment.

ISO 14040 and 14044 define four phases of an LCA, Goal and Scope Definition, Life Cycle Inventory (LCI), Life Cycle Impact Assessment (LCIA) and Interpretation of Results, which are described in the following paragraphs.

1. Goal and Scope Definition

This phase involves describing the problem, defining objectives, and outlining the scope of the investigation. It includes the definition of the functional unit, system boundaries, data availability, assumptions, and methodology limitations. The Functional Unit is a standardized measure that aligns with the study's goals and scope, facilitating the organization and presentation LCA data. It serves as a reference point for connecting energy and material flows and enables comparisons between different LCA studies. System Boundaries define the scope by specifying which processes and stages of the product's life cycle are included and excluded. These boundaries are organized into three parts: Upstream, Core, and Downstream, ensuring data quality for critical processes. Data availability refers to the ability of inventory data to accurately describe the emissions and environmental impacts of the system being modelled. Achieving good representativeness is especially crucial for significant processes. Assumptions and Limitations are necessary when there is missing information. Documenting the reasoning behind these decisions helps the audience understand the results more comprehensively. Clearly defining the objectives and scope is crucial to prevent misinterpretation of results.

2. Life Cycle Inventory (LCI)

Involves gathering information on the inputs and outputs of mass and energy flows per functional unit along the product value chain. Data collection and system modeling must align with defined objectives. LCI results serve as crucial input for the Life Cycle Impact Assessment (LCIA) phase.

3. Life Cycle Impact Assessment (LCIA)

Identifies and quantifies potential impacts of a product or process. Various impact assessment methods address impacts on human health, ecosystem quality, climate change, and resource depletion. LCIA translates LCI results into potential environmental impacts using characterization factors. Methods may focus on midpoint categories (e.g., IPCC, EDIP 2003) or both midpoint and

endpoint categories (e.g., IMPACT 2002+ and ReCipe). It includes several key steps: Classification involves categorizing inventory results according to impact categories, while Characterization involves transforming inventory data into category indicator scores using characterization factors. Normalization processes the data to obtain relative parameters based on reference values, facilitating accurate comparisons. Weighting evaluates the impact categories based on their importance by multiplying category indicators with numerical factors that reflect these considerations.

4. Interpretation of Results

This phase involves evaluating Life Cycle Impact Assessment (LCIA) results, identifying relevant issues, drawing conclusions, and formulating recommendations.

Economic aspect: Life Cycle Costing (LCC)

Life Cycle Cost (LCC) is “an assessment of all costs associated with the life cycle of a product that is directly covered by any one or more of the actors in the product life cycle (e.g., supplier, manufacturer, user or consumer, or EoL actor) with complementary inclusion of externalities that are anticipated to be internalized in the decision-relevant future (...)” (Hunkeler et al., 2008). This definition is considered as the current state of the art and starting point of LCA-type LCC. According to the Royal Institute of Chartered Surveyors (Gupta, 1983), the objectives of LCC are: (1) to enable investment options to be more effectively evaluated; (2) to consider the impact of all costs rather than only initial capital costs; (3) to assist in the effective management of completed buildings and projects; and (4) to facilitate choice between competing alternatives.

In literature, it is possible to find three types of LCC such as “conventional LCC”, “environmental LCC”, and “Societal LCC” (Menegaldo et al., 2023) (UNEP, 2011). Conventional Life Cycle Costing (LCC) includes private costs and benefits, while environmental LCC also considers external costs and benefits that are expected to be privatized in the future. For example, if there is an anticipated CO₂ tax or a future subsidy for hiring unskilled workers, these will be reflected in the LCC calculations. The third approach is called Societal LCC, where all private and external costs and benefits are monetized.

Currently, one widely recognized standard for performing a Life Cycle Cost (LCC) analysis is the (ISO 15686-5, 2017). However, this standard is specifically designed for LCC analyses of buildings and constructed assets. The primary objective of LCC, in general, is to evaluate the economic impacts across all stages of a product's life cycle. Therefore, four similar phases to that of Life Cycle Assessment (LCA) can be used to conduct an LCC: goal and scope definition, inventory costs, aggregation of costs by cost categories, and interpretation of results (UNEP, 2011). In the first phase, aspects such as the study's objective, the functional unit, specific system boundaries, and the life cycle actor's perspective (whether supplier, manufacturer, user, or consumer) are considered. During the second phase, costs are inventoried at the unit process level. In the third phase, the inventoried costs are aggregated by cost categories. Finally, in the fourth phase, the results are interpreted.

Social aspect: Social Life Cycle Assessment (S-LCA)

"Social Life Cycle Assessment (S-LCA) is a methodology used to evaluate the social impacts of products and services throughout their life cycle, from raw material extraction to the end-of-life phase, including disposal" (UNEP, 2020). S-LCA provides valuable information on social and socio-economic aspects to support decision-making, enhance an organization's social performance and ultimately improve the well-being of stakeholders.

As for the LCC, also the S-LCA methodology follows the Goal and Scope definition, Life Cycle Inventory, Life Cycle Impact Assessment, and Interpretation phases. In the first phase, the objective and scope of the study are established, including the purpose, expected use of results, target audience, functional unit, system boundaries, and assumptions made. In the second phase, data is collected to account for all social and socio-economic inputs and outputs associated with the product system. The data can be sourced from various references, including databases, reports, and literature. The Social Hotspot Database (SHDB) is often used to identify and assess social risks, and it has been used for SimaPro. The SHDB considers 25 impact subcategories and five aggregated impact categories. These are evaluated through 160 social impact indicators, such as the Child labour indicator. The SHDB uses the Social Hotspot index to express social risk in medium risk hours equivalent (mrheq), calculated by multiplying the working hours data by the risk level, which ranges from very high to low. In the third phase, Life Cycle Impact Assessment, the potential social impacts identified during the LCI phase are assessed. While conducting a S-LCA two approaches can be

followed, Reference Scale Assessment (RS S-LCA) and Impact Pathway Assessment (IP S-LCA). RS S-LCA evaluates social performance or risks, while IP S-LCA links social consequences in cause-effect relations. The SHDB offers the functional reference scale method for SimaPro, developed by NewEarth B company, to estimate social risk probability. Risk levels vary from very high to low, with associated characterization factors converting data into mrheq. In the interpretation phase, results are thoroughly analyzed, summarized, and discussed to produce a final assessment with conclusions, recommendations, and information for decision-making steps.

1.3.SUNSHINE project and case studies

SUNSHINE is an industry-oriented project started in January 2021 and finished in December 2024, where leading research and technology organisations cooperated with SMEs and large industries to develop and implement simple, robust and cost-effective SSbD strategies for materials and products incorporating MCNMs. To this end, the project established a user-friendly e-infrastructure to foster dialogue, collaboration and information exchange between actors along entire MCNMs supply chains. SUNSHINE's aims were to transform the state-of-the-art knowledge, tools and data on the exposure and hazard characteristics of MCNMs, especially those arising from their unique properties, into SSbD strategies implementable at industrial scale. The SSbD strategies aim to modify materials, products and processes to reduce the potential for release of MCNMs, accelerate their degradation in physiological or environmental media, and/or decrease their persistence, bioaccumulation and/or hazard. To propose effective strategies, the SUNSHINE SSbD tiered approach has been developed and applied to different case studies for identifying safety, sustainability and functionality hotspots. Its applications addressed different objectives: (i) testing on different cases within SUNSHINE (i.e., anti-sticking coating and active food packaging), (ii) testing on an external case in the context of a specific collaboration (i.e., ACRE TFT), and (iii) comparison to Early4AdMa Tier 2; in this case both approaches have been tested to another SUNSHINE case study (i.e., innovative flame retardant).

The four case studies to which the approach has been applied are explained in the paragraphs below.

Anti-sticking coating

The first case study introduced a MCNM coating made of silica carbide and titanium dioxide (SiC@TiO_2), which offers non-stick properties for applications such as bread baking trays. This

innovative material serves as an alternative to PFAS-based non-stick coatings, like Teflon®. PTFE is extensively utilized across various industries due to its chemical, thermal, and electrical stability, as well as its low friction properties (Sajid & Ilyas, 2017). Teflon® which is the considered benchmark for this study, can be employed as a coating material in non-stick cookware to prevent food from adhering during cooking. However, at typical cooking temperatures, PTFE-coated surfaces release chemicals and gases that range from mild to severely toxic. Furthermore, the synthesis of PTFE involves the use of PFOA (perfluorooctanoic acid), a well-known environmental pollutant, and there are reports of PFOA being detected in the gas phase emitted from cooking utensils under normal cooking conditions (Sajid & Ilyas, 2017). Since exposure to elevated levels of certain PFAS causes adverse health effects, since they are suspected carcinogens (Stewart & Wild, 2014), there is a concerted effort within industries to identify safer and more sustainable alternatives to these type of materials. Eliminating the use of toxic and carcinogenic substances such as PFAS represents a significant advancement towards safer products. For this reason, Laurentia realized a Sol-Gel-Derived Silicon-Containing Hybrids modified with SiC@TiO₂, which enhance anti-sticking properties when used as coatings on baking trays. The MCNM comprises two material components: a 60nm SiC@TiO₂ and a 500nm SiC@TiO₂. The presence of SiC enhances the material mechanical and thermal properties, durability, and anti-sticking capabilities (Pizzol et al., 2023). In the thesis titles and subtitles, the case study will be referred to as 'Anti-sticking coating' instead of 'anti-sticking coated baking trays' for the sake of brevity.

Active food packaging

The second case study develops, produces and markets active food packaging that is intended to improve food safety, extend food self-life and accelerate biopolymer biodegradation when the packaging is discarded after use. The company that produces the material detects an opportunity to active food packaging that prevents infection by food insect pests. The material provided by the company and assessed for this case study is made of nano drops of essential oil anchored to the surface of nano clays and encapsulated in a polymeric film. Specifically, this innovative product must also satisfy food contact regulatory and biodegradation issues. This innovative material is a substitute for Low-Density Polyethylene (LDPE) and it's produced to develop food packaging to keep the

packaged food free of insect pests. Indeed, it is well known that the incorporation of essential oil in thermoforming polymers is not possible because the process temperatures used in forming are higher than the decomposition temperatures of essential oils (Pizzol et al., 2023). Moreover, the polymer originated from non-renewable sources as fossil fuels are not able to be biodegraded in compost after packaging disposal. Therefore, in addition to the new functionality the industries are currently searching for ways to substitute LDPE food packaging for safer and more sustainable alternatives. The material produced by the company consists of a MCNM of nano drops of essential oil (clove oil food grade) anchored on the nano clays (E-558 bentonite clay as layered nano clay; E-562 sepiolite as fibrillary nano clays) that are first encapsulated by an organic acid (E-297 Fumaric acid) and therefore incorporated into the polymeric matrix (second encapsulation) during the thermoforming of the food packaging (Salgado et al., 2023 Patent application: EP23382230.3). All the components of the MCMM are based on food grade or food additive materials and the process is free of other chemicals or solvents that are not allowed in the food contact regulation.

The considered benchmark is LDPE, the most common packaging material used for packaging a wide range of products (Veethahavya et al., 2016). LDPE is defined by a density range of 0.910–0.940 g/cm³ and it can withstand temperatures of 80 °C continuously and 95 °C for a short time. LDPE is quite flexible and tough, indeed, it is used to package foods, milk, agricultural products, shrink-wrapping, electronic goods, vehicles, and so on. (Veethahavya et al., 2016)

ACRE TFTs

As previously mentioned, this case study is external to the SUNSHINE project. However, it is linked to SUNSHINE via the collaboration between SUNSHINE and the project INFRAMES, which includes both SUNSHINE and Duke University. Duke University has provided the case study currently being evaluated. Specifically, the material under assessment is being developed within the *LEAP-HI: All-Carbon Recyclable Electronics (ACRE) Realizing a Sustainable Electronics Lifecycle* project, which focuses on discovering and developing all-carbon recyclable electronic materials, such as thin film transistors (TFTs). Typically, a transistor is made up of various components constructed from silicon- or metal oxide-based semiconductor materials. For an ACRE transistor, however, these components are replaced with materials in ink form, such as crystalline nano-cellulose (CNC), carbon nanotubes

(CNT), and graphene. By utilizing carbon-based materials, the project aims to significantly reduce emissions associated with electronic manufacturing processes. Indeed, the production of semiconductor components causes the usage of various acid/base solutions, organic solvents, and toxic gases releasing highly polluting toxins, wastewater, and waste gas (F. Lin et al., 2019). Additionally, the manufacturing processes of silicon- or metal oxide-based semiconductor materials for devices like flat-panel displays are known to release high levels of greenhouse gases (GHGs) into the atmosphere. Indeed, the semiconductor industry makes up 1.3–2.0% of the overall electricity usage in the manufacturing sector in the US. (Kuo et al., 2022). The LEAP-HI project specifically aims to replace silicon- or metal oxide-based semiconductor materials and their high greenhouse gas (GHG) emitting manufacturing processes, particularly in the flat-panel display industry. Electronic display backplanes are a promising target for printed nanomaterials to revolutionize, as the required performance for these devices is within reach, and the need to reduce high-GHG manufacturing is substantial.

Innovative flame retardant

This case study develops, produces, and markets high-performance nanomaterials and nanotechnology-based solutions. Specifically, is specialized in the development, production and commercialization of specialty additives for different materials, mainly plastics and rubber, across different industries: automotive, aeronautics, safety equipment, footwear, painting, building, wire and cable sector, fabrics, packaging and paper, among others. The material provided by the company and assessed for this case study is a nanocomposite of graphene oxide functionalized with chitosan. This nanocomposite is then embedded on a surface as polyurethane or polyamide. This innovative material is a substitute for conventional flame retardants such as melamine cyanuric acid. Indeed, the technologies used nowadays to obtain fireproof fabrics are based on compounds that release both halogens, antimony trioxide and formaldehyde, which present health problems and environmental impacts (Nora et al., 2020).

2. Chapter 2 Methods

In this chapter, the methodologies employed to develop the SUNSHINE SSbD approach are presented in detail, alongside the approach itself, structured into two distinct tiers. Additionally, the chapter includes an in-depth look at the methodology used to compare Tier 1 of the SUNSHINE SSbD approach with Tier 2 of the Early4AdMa approach. The application of the SUNSHINE SSbD approach is then demonstrated in Chapter 3, "Results," through a series of case studies showcasing its practical implementation and effectiveness in addressing the research objectives.

2.1. The SUNSHINE SSbD approach

Following the adoption of the EC's SSbD Framework, in the context of the SUNSHINE project, a tiered approach has been developed. The reason for adopting different tiers for the assessment stems from considerations that the information available for newly developed chemicals or materials could be limited in the early stages of development (e.g., R&D stage), while availability of data and expertise increases in the later product development and optimization stages, which also demand more thorough assessment of safety and sustainability.

The proposed SSbD approach is implemented in two levels of assessment as reported in Figure 1. It is a tiered approach with each tier increasing the complexity of the employed assessment methods as well as the time, resources, data and level of expertise required for their application. Hence, the first level evaluates safety and sustainability through qualitative methods (Tier 1) while the second level evaluates safety and sustainability through quantitative methods (Tier 2).

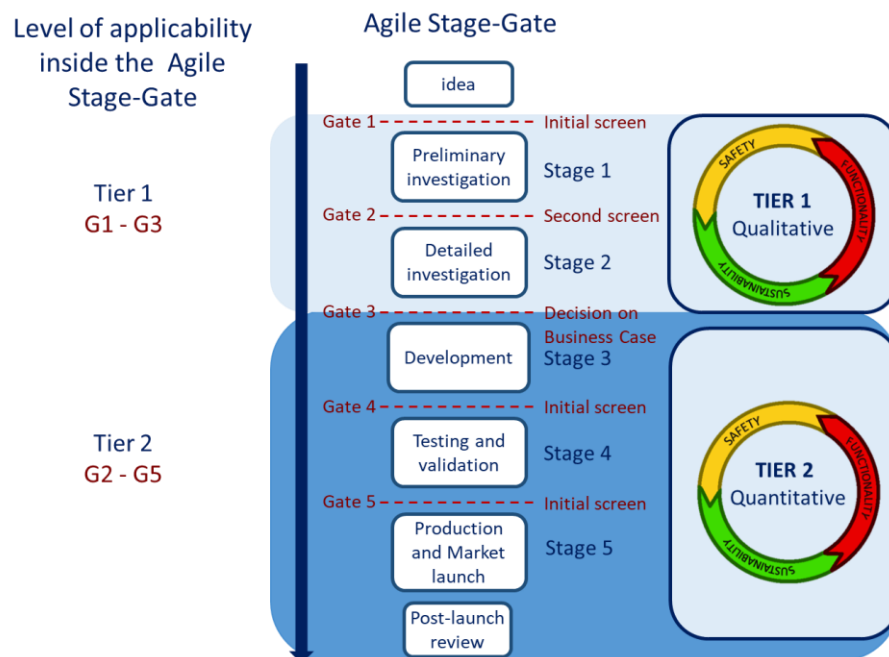


Figure 1 SSbD tiered assessment proposed in the SUNSHINE project. ‘Level of applicability’ means at which gate of the stage-gate the approach can be applied.

Tier 1 is applied at the screening level in the early stages of innovation, while Tier 2 is applied at a more advanced level when the products are already developed and are ready to be released on the market. The proposed SUNSHINE SSbD tiered approach has been aligned to the Agile Stage-Gate innovation model (Cooper, 2014; Cooper & Sommer, 2018). Agile Stage-Gate is a standard industrial approach that divides the innovation process into five Stages and requires analysis at each Gate to inform decisions on: (1) Termination if the technical or commercial probability of success are compromised, or if the EHS risks are considered unacceptable; (2) Stage reiteration to improve the safety, performance and/or sustainability of the material/product being developed; or (3) progression to the next Stage if those are in the desired ranges. In this way, the Agile Stage-Gate approach continuously challenges the early stages of innovation to develop safer, functional and more sustainable products cost-efficiently.

Specifically, Tier 1 involves qualitative self-assessment analysis by the industry at the very early stages of the innovation process that aims to identify hotspots (i.e., the sources of potential impacts, such as the emissions to air, along the life cycle) of possible safety and/or sustainability issues to take actions before more resources are invested into further developing the product. Hence, a

questionnaire for pre-evaluation of safety, sustainability and functionality is proposed, which can be applied to qualitatively assess possible design alternatives (that are hypothesised or known to be technologically functional) to inform the selection of best options for developing safer and more sustainable materials/products. For the safety aspect, questions have been defined according to the steps of the risk assessment methodology, which includes hazard identification, exposure assessment and risk characterization. Specifically, information about toxicity, genotoxicity, and toxicokinetic needs to be investigated for advanced materials according to EFSA guidance (Scientific Committee et al., 2021). Also, based on the substance evaluation process of the REACH Regulation, it is possible to identify which “Initial grounds of concern” (e.g., suspected carcinogenic, other hazard-based concern, consumer use, exposure of workers) can influence the hazard to human health and environment and therefore need to be investigated. Concerning environmental sustainability, questions were defined according to the “environmental impact categories” used within the LCA methodology, as indicators of specific impacts on the environment (e.g., potential global warming potential, acidification of soils and water, depletion of natural non-fossil resources). For social sustainability, questions were asked according to the social impact categories, which are used with S-LCA methodology to quantitatively investigate the social impacts of organisations and products. For economic sustainability, questions were proposed with the aim of understanding if the necessary information to perform an LCC is available for the product under assessment. Finally, for the functionality aspect, questions were defined to identify characteristics making a product functional by its design. Indeed, functional design is the process of formulating a unique design problem by mapping customer needs onto a set of functional requirements (Liu & Lu, 2020).

The proposed SSbD approach is always comparative as it enables to assess if a modified MCNM or the respective product performs better in terms of safety, functionality and performance than another SSbD design alternative or than a conventional material/product that has the same or a similar function. Tier 2 consists of the REACH Chemical Safety Assessment (CSA) approach and Life Cycle Sustainability Assessment (LCSA) methodologies, but the CSA is out of the scope of this thesis, which only focuses on Steps 4 and 5 of the EC-JRC, namely Life Cycle Assessment (LCA), Life Cycle Costing (LCC) and Social Life Cycle Assessment (S-LCA).

For higher tiers, as Tier 2 of the SUNSHINE SSbD approach, some SSbD approaches are already available in the literature. These have been applied to assess the sustainability of indigo dyeing color in the fashion sector (Lai & Chang, 2021) or of inhibitors in pharmaceutical products (Romeiro et al., 2019), the design of cellulosic bioelectricity supply chain networks (Yue et al., 2014), the design of a commercial building in Shanghai (Wang et al., 2010) and the sustainability of mechatronic systems application to a regenerative braking system (Mehdi & Boudi, 2021). In the case of lower tiers of assessment few methodologies are available, one examples is the one developed by (Schmidt Rivera et al., 2019) for innovative and sustainable food packaging.

The early R&D stage of chemical and material development is crucial in the innovation process. To address this gap, this thesis introduces an SSbD approach designed to compare design alternatives through two complementary tiers: a pre-evaluation questionnaire, suitable for scenarios where only limited qualitative information is available, and LCSA methodologies for conducting comprehensive evaluations when quantitative data is accessible. These are integrated into a unified approach intended for continuous application throughout the design stages, enabling ongoing analysis of the product under development. This ensures that potential hotspots are identified and resolved proactively, long before the product enters the final stages of the stage-gate process, where substantial financial investments have already been made. While Tier 2 is based on standardized methodologies, Tier 1 was developed through iterative steps in collaboration with key stakeholders from various fields, ensuring it is representative and well-suited for assessing safety and sustainability effectively.

2.2.Tier 1

The methodological steps for the development of the self-assessment questionnaire representing Tier 1 of the SUNSHINE approach are reported in Figure 2. First of all, a first series of questions was identified in co-creation with key stakeholders (S.H.) from industry, regulation, policy, academia, all inspired by “Safe and Sustainable by Design chemicals and materials: Framework for the definition of criteria and evaluation procedure for chemicals and materials” (Step 1) (C. Caldeira et al., 2022). Moreover, a working group of experts in developing Frameworks for SSbD and risk assessment of NMs from EU projects, along with experts in environmental and socio-economic sustainability, was

set up, which periodically met to frame the questionnaire and identify the relevant questions (Step 2).

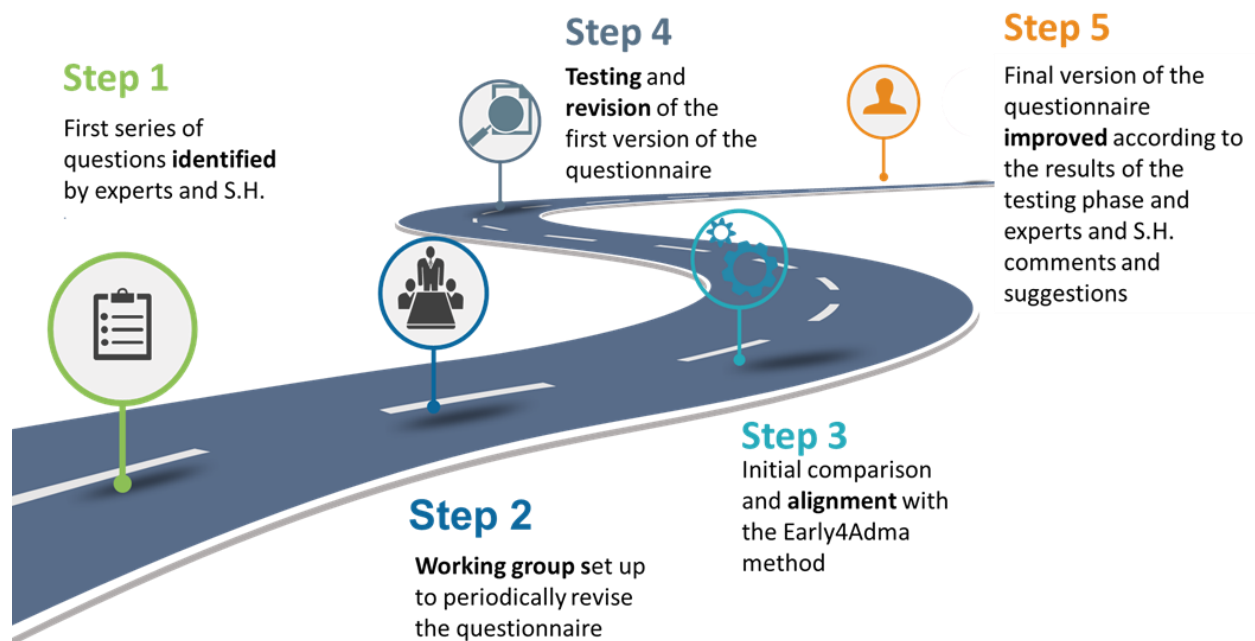


Figure 2 Methodological steps to develop the questionnaire in Tier 1.

These questions were targeted at innovators from industry, especially SMEs, and were aligned with the questions of “Towards Safe and Sustainable Advanced (Nano)materials: A proposal for an early awareness and action system for advanced materials (Early4AdMa)” (Step 3) (Oomen et al., 2022), which, in contrast, targets regulators and policymakers. The scope of the questions of the proposed self-assessment methodology addresses the safety, functionality, and sustainability of advanced materials, with a special focus on socioeconomic aspects. On that basis, a first version of a questionnaire was released and tested in the case studies of the SUNSHINE project (Step 4). The results were further discussed and elaborated so that the questions related to the safety and functionality aspects were improved, thanks to a stronger collaboration with industries and experts in regulatory risk assessment. The questions about socioeconomic aspects were improved through the alignment with the categories and subcategories provided by the approach described previously (Stoycheva et al., 2022) and the UNEP methodological sheets (Step 5)(UNEP, 2021)

In the final version of the questionnaire, the experts decided which questions were relevant for screening of safety, sustainability, and functionality along five life cycle stages (LCS): i.e., (1) Raw materials and resources needed to produce the material/product, (2) Production of the MCNM, (3) Production of the product incorporating the MCNM, (4) Use of the product, and (5) End of Life (EoL) treatment.

Regarding the safety dimension, the eventual presence of hazardous materials, such as carcinogenic, genotoxic, endocrine-disrupting materials, and the physical hazard properties of the MCNM were investigated along the LCS. At the same time, the release and emission of hazardous substances due to the production of the MCNM and the related enabled product, e.g., the possible release of carcinogenic, persistent, bioaccumulating substances from the product, and the transformations of any released MCNM, were also assessed along the LCS.

Regarding the environmental sustainability dimension, the use of critical and/or renewable materials, the energy sources, the use of water, as well as consideration related to generation of waste and greenhouse gases (GHG) emissions, chemical emissions in environmental compartments, possibility to recycle the waste generated during the production process and reusing any by-products/co-products were investigated.

For the social sustainability dimension, the following aspects were addressed: respect of the living conditions of affected local communities, the policies and restrictive procedures for the traceability of raw materials, minimization of social issues related to the acquisition of raw materials and resources, the promotion of regional products, the social responsibility of suppliers, the technological development and educational opportunities, and the screening of possible End of Life treatment options.

Regarding the economic sustainability dimension, the provision of the costs of the raw materials and their transport, the materials production, products manufacturing and waste disposal, the installation costs for implementing SSbD actions, the direct economic benefits in using the innovative product and the direct costs of the End-of-Life treatment were considered.

Finally, for the functionality dimension, characteristics such as durability, reliability, usability, and versatility were investigated in Use LCS.

On the basis of the consideration reported above, the developed questionnaire is divided into four parts, where the first part is an introduction to the proposed SSbD approach and explains the goal and scope of the survey, as reported in Annex 1.

The second part (Table 23 in Annex 2) consists of general questions related to both the MCNM and the respective product. These questions investigate the products' functionality, the sector of application and identify a benchmark against which the assessed product can be compared. These questions are intended to obtain a general idea of the target material/product and to pinpoint to possible hotspots (sources) of potential health or environmental impacts. These hotspots would then be assessed in more detail in the subsequent Tier 2.

In Table 23 in Annex 2 general questions related to the MCNM and the respective product are considered, while Table 24 in Annex 2, the third part of the questionnaire, is aimed at collecting a set of information about the MCNM and the product incorporating the MCNM during the remaining stages: production, use and end-of-life.

Specifically, inputs, such as chemicals, energy sources, and water use, and outputs, such as waste, and emissions, are required, since they can cause impacts in terms of global warming, eutrophication, acidification of water, etc., with an inevitable negative effect on human health and the environment. Furthermore, additional questions are asked to obtain information on aspects of sustainability and functionality such as for example the recycling/re-use options within a circular economy perspective or key critical quality attributes, and the yield of the production process. The questions related to the Use stage are asked to understand the lifetime of the material/product, if the company is aware of how it wants to increase its sustainability during the Use stage, and who is the final client/customer. Finally, the questions related to the End of Life are asked to understand both, if the company has considered the idea of producing biodegradable, recyclable, and reusable materials/products, if transformations are expected during the End of Life and if the company has considered different End of Life alternatives.

The second and third part of the questionnaire are not comparative, indeed their aim is not to compare the designed alternatives but to help the user to collect the data needed to fulfil the fourth part of the questionnaire. Accordingly, the structure of these two parts is the same of the fourth.

The fourth part of the questionnaire is more specific and includes a set of detailed questions that need to be considered during the R&D stage. The possible answers to each question are “Yes”, “No”, “I don’t know” and “Not applicable”. The assessment is performed by comparing either the material/product against a benchmark (i.e., another existing material/product which has the same function) or the alternative modification options (e.g., different coatings).

Basing on the type of question, “Yes” and “No” answers are associated to positively or negatively contributing to safety and sustainability, e.g., answering “Yes” to “Are any of the raw materials carcinogenic?” results in a negative contribution as opposed to answering “Yes” to “Do you use renewable raw materials?” which results in a positive contribution. The questionnaire aims to establish which of the compared alternatives have the highest number of answers with positive contributions to sustainability, regardless of the actual “Yes” or “No” answer.

This simple comparison is complicated by the presence of uncertain answers (i.e., I don’t know) which make the results of the comparison itself uncertain, i.e., it is not possible to state that one solution is contributing to sustainability more than another, but rather that it has a certain probability of doing so. As each uncertain question can only take two possible states, “Yes” or “No”, it can be seen as a Bernoulli trial (Proakis, 1985). When considering the whole set of uncertain questions, the result’s probability distribution is therefore modelled by a binomial distribution (i.e., the probability distribution of a sequence of a specific number of independent Bernoulli trials with fixed success probability).

As the aim of the questionnaire is to establish which of the compared alternatives have the highest number of answers with positive contribution to sustainability this implies comparing the results of different Binomial distributions, one for each alternative, and establish how likely it is that one alternative has a higher number of positive contributions than the other. To do so, for each alternative, the starting number of answers with a positive contribution is used as a fixed base upon which the Binomial distribution’s possible outcomes are summed. Then, each possible result of the

target material/product is compared against each possible result of the other scenarios and the conjunct probabilities of all the pairs of results for which the innovative target alternative beats the other are summed up.

To avoid the possible biases related to the number of 'Not applicable' answers, results are expressed as percentages of positives as opposed to the absolute number of positives. This also allows comparisons between products with a different number of not applicable responses.

The presented methodology has been implemented in a Microsoft Excel tool, which automatically compares the alternatives and produces results and charts.

The fourth part is divided into five sections which represent the five LCS assessed during the R&D stage: 1) Raw materials and resources needed to produce the material/product, 2) Production of the MCNM, 3) Production of the product incorporating the MCNM, 4) Use of the product, and 5) End of Life treatment. This subdivision was made to obtain information on all phases of the product life cycle, starting from the extraction of raw materials, up to the EoL management. For each of the five LCS, the set of questions/issues to be addressed are divided according to the following classifications: the aspects to be considered (e.g., safety, functionality and economic, environmental and social sustainability aspects), the ambitions to be reached, the objectives/criteria which describe the fulfilment of the identified ambitions, and the indicators and the questions used to measure the fulfilment. In the next sections, the detailed description of the fourth part of the questionnaire is presented for each lifecycle stage.

2.2.1.Raw materials and resources needed to produce the material/product

This section shows how the stage of raw materials and resources is addressed and considered within Tier 1 for the case studies at hand. There are thirty questions in this section, twenty for the first group (safety) and ten for the second group (environmental, social and economic sustainability) (Table 1).

Table 1 Aspects, Indicators and Questions related to the Raw materials and resources stage.

Aspects	Indicators	Questions
Safety	Chemical components included in authoritative lists	Are any of the chemical components used to produce the MCNM* included in any authoritative lists of restricted and

Aspects	Indicators	Questions
		hazardous chemicals (e.g. candidate list of SVHC according to Article 57 of REACH)?
	Carcinogenic raw materials	Are any of the raw materials carcinogenic?
	Genotoxic raw materials	Are any of the raw materials genotoxic (mutagenic)?
	Toxic raw materials	Are any of the raw materials toxic to reproduction?
	Endocrine disrupting properties raw materials	Do any of the raw materials have endocrine disrupting properties relevant to human health?
	Respiratory sensitiser raw materials	Are any of the raw materials a respiratory sensitiser?
	Specific target organ toxicity raw materials	Do any of the raw materials have specific target organ toxicity?
	Immunotoxic raw materials	Are any of the raw materials immunotoxic?
	Neurotoxic raw materials	Are any of the raw materials neurotoxic?
	Skin sensitiser raw materials	Are any of the raw materials a skin sensitiser?
	Raw materials that have adverse effects on eye/skin	Do any of the raw materials have adverse effects on eye/skin (e.g. eye damage/irritation, skin corrosion/irritation)?
	Acute toxicants raw materials	Are any of the raw materials acute toxicants?
	Persistent raw materials	Are any of your raw materials persistent, mobile and toxic (PMT) or very persistent and mobile (vPvM)?
	(Acute) ecotoxic raw materials	Are any of the raw materials (acute) toxic to the environment?
	(Chronic) ecotoxic raw materials	Are any of the raw materials (chronic) ecotoxic?
	Hazardous to the ozone layer raw materials	Are any of the raw materials hazardous to the ozone layer?
	Bioaccumulative raw materials	Are any of your raw materials bioaccumulative?
	Endocrine-disrupting properties raw materials	Do any of the raw materials have endocrine-disrupting properties relevant to the environment?
	Physical hazard properties raw materials	Do any of the raw materials have physical hazard properties (explosive, flammable, corrosive, etc.)?
	Fiber like raw materials	Do any of your raw materials contain fibre like materials (i.e aspect ratio ≥ 3)
	Critical materials	Are critical materials used? See EU List

Aspects	Indicators	Questions
Environment sustainability	Use of raw materials derived from renewable resources	Do you use renewable raw materials?
Social sustainability	Material resources access	Do your suppliers respect and protect community access to local material resources (i.e., water, land, mineral, and biological resources) and infrastructure (i.e., roads, sanitation facilities, schools, etc.)?
	Health and safety improvement	Does the activity contribute to improvements to (e.g., through sharing health services) the safety and health of the local community?
	Health and safety improvement	Does the activity contribute to damage (e.g., use of hazardous materials, pollution) to safety and health of the local community?
	Traceability of raw materials	Are there policies in place to allow traceability of your raw materials?
	Absence of armed conflicts	Is the origin country of raw materials free from armed conflicts?
	Raw materials coming from underdeveloped, developing or third world countries	Are there restrictive procedures to minimise social issues (e.g., child labour, political or demographic problems, poor working conditions, forced labour, unfair salary, inequality, etc)?
Economic sustainability	Direct costs for raw material	Can you provide the costs of your raw materials?
	Direct costs of transportation for raw materials	Can you provide the costs of the transport of your raw materials?

* As the questionnaire is of a comparative nature, the term MCNM is considered when assessing the MCNM. The term MCNM is replaced by the term benchmark when the benchmark is assessed

2.2.2. Production of the MCNM

This section shows how the stage of the Production of MCNM is addressed and considered within Tier 1. As reported in

Table 2, there are forty-nine questions, twenty-six for the first group (safety) and twenty-three for the second group (environmental, social and economic sustainability).

Table 2 Aspects, Indicators and Questions related to the Production of the MCNM stage.

Aspects	Indicators	Questions
Safety	Chemical components included in authoritative lists	Is the MCNM* in any authoritative lists of restricted and hazardous chemicals (e.g. candidate list of SVHC according to Article 57 of REACH)?
	Carcinogenic MCNMs	Is the MCNM* carcinogenic?
	Genotoxic MCNMs	Is the MCNM* genotoxic (mutagenic)?
	Toxic MCNMs	Is the MCNM* toxic to reproduction?
	Endocrine-disrupting properties of MCNMs	Does the MCNM* have endocrine-disrupting properties relevant to human health?
	Respiratory sensitiser MCNMs	Is the MCNM* a respiratory sensitiser?
	Specific target organ toxicity MCNMs	Does the MCNM* have any specific target organ toxicity?
	Immunotoxic MCNMs	Is the MCNM* immunotoxic?
	Neurotoxic MCNMs	Is the MCNM* neurotoxic?
	Skin sensitiser MCNMs	Is the MCNM* a skin sensitiser?
	MCNMs that have adverse effects on eye/skin	Does the MCNM* have adverse effects on the eye/skin (e.g. eye damage/irritation, skin corrosion/irritation)?
	Acute toxicants MCNMs	Does the MCNM induce acute toxicity?
	Persistent MCNMs	Is the MCNM* persistent, mobile and toxic (PMT) or very persistent and mobile (vPvM)?
	(Acute) ecotoxic MCNMs	Does the MCNM* induce any acute environmental toxicity?
	(Chronic) ecotoxic MCNMs	Does the MCNM* induce any chronic environmental toxicity?
	Hazardous for the ozone layer MCNMs	Is the MCNM* hazardous to the ozone layer?
	Bioaccumulative MCNMs	Is the MCNM bioaccumulative?
	Endocrine disrupting properties MCNMs	Does the MCNM* have endocrine disrupting properties relevant to environment?
	Physical hazard properties MCNMs	Does the MCNM* have any physical hazard properties (explosive, flammable, corrosive, etc.)?
	Fibre like MCNMs	Is the MCNM* a fibre-like materials (i.e high aspect ratio ≥ 3)
	Active routes of exposure for workers	Are there any active routes of exposure for workers that can be expected during the production of the MCNM*?

Aspects	Indicators	Questions
	Occupational exposure and upscaling process	Will occupational exposure increase due to the upscaled process?
	Chemical or NM emission	Are there any chemical or NM emissions into the indoor environment?
	Dustiness from the production process	Does the production process produce dust?
	Liquid emission from the production process	Does the production process cause leaks or releases of liquids?
	NM emissions into the environment	Are there any chemical or NM emissions into the environment? (wastewater and airborne)
Environment sustainability	Critical materials	Are other critical materials used? See EU List
	Consumption of water resources in the production process	Are you in the process of reducing water consumption during the production process?
	Increase the yield of your process	Are you in the process of increasing the yield of your process?
	Reduce the use of raw materials	Are you in the process of reducing the raw materials use?
	Impact on climate change from the production process	Are you in the process of reducing greenhouse gases when producing your innovative material?
		Are renewable energy resources used?
	Energy consumption during the production process	Are you in the process of reducing the energy consumption when producing your innovative material (for instance, considering different temperatures and reducing the pressure)?
	Emissions to water	Are you in the process of reducing the emissions of chemicals and of NM to water generated during the production process?
	Emissions to the air	Are you in the process of reducing the emissions of chemicals and of NM to the air generated during the production process?
	Waste production during the production process	Are you in the process of reducing the waste generated during the production process?
	Reuse of by-product/co-product	Are you in the process of re-use the by-products/co-products generated during the production process?
	Recyclability of waste produced in production process	Are you in the process of recycling the waste produced during the production process?

Aspects	Indicators	Questions
Social sustainability	Health and safety improvement	Does the activity contribute to improvements to the (e.g. through sharing health services) safety and health of the local community?
	Health and safety improvement	Does the activity contribute to damage (e.g. use of hazardous materials, pollution) safety and health of the local community?
	Local employment	Does the organization positively affect the local employment rates?
	Assessment of suppliers	Are suppliers socially responsible (e.g. if they implement CSR principles)?
	Raw materials coming from underdeveloped, developing or third world countries	Are there restrictive procedures to minimise social issues (e.g., child labour, political or demographic problems, poor working conditions, inequality. etc)?
	Technological development, economic impact, education opportunities	Did you consider if the production process results in technological development, additional education opportunities?
Economic sustainability	Direct costs of waste disposal in production	Can you provide and/or estimate the costs of disposable waste during material production?
	Direct costs of maintenance for production	Can you provide and/or estimate the costs of the material production process?
	Direct costs of installation (heating, lighting) for production	Are installation costs expected for implementing SSbD actions?
	Economic benefits of by-product/co-product	Can you sell your by-product/co-product?
	Direct benefits of production	Can you identify direct economic benefits for the innovative material?

* As the questionnaire is of a comparative nature, the term MCNM is considered when assessing the MCNM. The term MCNM is replaced by the term benchmark when the benchmark is assessed

2.2.3. Production of the product incorporating the MCNM

This section shows how the stage of the production of the product that incorporates the MCNM is addressed and considered within the Tier 1. As reported in Table 3, the questionnaire contains twenty-nine questions, eleven for the first group (safety) and eighteen for the second group (environmental, social and economic sustainability).

Table 3 Aspects, Indicators and Questions related to the Production of the product incorporating the MCNM stage.

Aspects	Indicators	Questions
Safety	Active routes of exposure for workers	Are there any active routes of exposure for workers that can be expected during the production of the product incorporating the MCNM*?
	Occupational exposure and upscaled process	Will the occupational exposure increase due to the upscaled process?
	Chemical or NM emission	Are there any chemical emissions into the indoor environment?
	Dustiness from the production process	Does the production produce dustiness?
	Liquid emission from the production process	Does the production process emit liquid emission?
	Release of bioaccumulating substances	Does your production process release bioaccumulating substances?
	Exposure reduction measures	Do you put in place exposure reduction measures to produce the product incorporating the MCNM*?
	Release of persistent substances	Does your production process release persistent substances?
	Release of carcinogenic substances	Does your production process release carcinogenic substances?
	Release of suspected carcinogenic substances	Does your production process release suspected carcinogenic substances?
	NM emissions into the environment	Are there any chemical or NM emissions into the environment?
Environment sustainability	Consumption of water resources in manufacturing	Are you in the process of reducing the water consumption during manufacturing?
	Impact on climate change (LCA midpoint) from manufacturing and production process	Do you use renewable energy resource during manufacturing?
	Impact on climate change from manufacturing	Are you in the process of reducing the emission of greenhouse gases when designing your innovative product?
	Energy consumption during manufacturing	Are you in the process of reducing energy consumption when designing your innovative product?

Aspects	Indicators	Questions
	Emissions to water	Are you in the process of reducing emissions of chemicals and of NM to water generated during manufacturing?
	Emissions to air	Are you in the process of reducing emissions of chemicals and of NM to air generated during manufacturing?
	Waste production during manufacturing	Are you in the process of reducing the waste generated during manufacturing?
	Reuse of by-product/co-product	Can you re-use or sell the by-product/co-product generated during the production process?
	Recyclability of waste produced in manufacturing	Are you in the process of making recyclable the waste produced during the manufacturing be recycled?
Social sustainability	Local employment	Does the organization positively affect the local employment rates?
	Assessment of suppliers	Are suppliers socially responsible (e.g., if they implement CSR principles)?
	Raw materials coming from underdeveloped, developing or third world countries	Are there restrictive procedures to minimise social issues (e.g., child labour, political or demographic problems, forced labour, unfair salary, poor working conditions, inequality. etc)?
	Technological development, economic impact, education opportunities	Did you consider if the manufacturing process results in technological development, additional education opportunities?
Economic sustainability	Direct costs of waste disposal in manufacturing	Can you provide the costs of disposal of waste during product manufacturing?
	Direct costs of water treatment for manufacturing	Can you provide the costs of water treatment for product manufacturing?
	Direct costs of maintenance for manufacturing	Can you provide the costs of the maintenance for product manufacturing?
	Direct costs of installation (heating, lighting) for manufacturing	Are installation costs expected for implementing SSbD actions?
	Direct benefits of product	Can you identify direct economic benefits for the innovative product?

** As the questionnaire is of a comparative nature, the term MCNM is considered when assessing the MCNM. The term MCNM is replaced by the term benchmark when the benchmark is assessed*

2.2.4. Use of the product

This section shows how the stage of the use of the product incorporating the MCNM is addressed and considered within Tier 1, assuming that the MCNM does not have a use without being incorporated in a product. In the cases when the MCNM have a use without being incorporated in a product, the provided questions can be adapted to the specific case. As reported in Table 4, there are forty-two questions in this section, nine for the first group (safety), thirteen for the second group (environmental and economic sustainability) and twenty for the third group (functionality).

Table 4 Aspects, Indicators and Questions related to the Use of the product stage.

Aspects	Indicators	Questions
Safety	Release of materials/substances that look like asbestos	Does your product release materials/substances that are fibre like (i.e., aspect ratio ≥ 3)
	Release of persistent substances	Does the product incorporating the MCNM release persistent substances during the use phase?
	Release of carcinogenic substances	Does the product incorporating the MCNM release carcinogenic substances during the use phase?
	Release of suspected carcinogenic substances	Does the product incorporating the MCNM release suspected carcinogenic substances during the use phase?
	Release of bioaccumulating substances	Does the product incorporate the MCNM release bioaccumulating substances during the use phase?
	Chemical or NM emission	Are there any release of MCNM* or of chemical into the environment?
	Physical hazard properties MCNMs	Does the product have any physical hazard properties (explosive, flammable, corrosive, etc.)?
	Reactivity of the MCNM	Do you expect that the MCNM* could be modified (transformed or degraded) during the use phase?
	Release of MCNM	Do you expect that the MCNM* could be released or dissolved from the matrix during the use stage?
Environment sustainability	Consumption of water resources in product use	Did you consider reducing water consumption when designing the use of your innovative product?
	Impact on climate change from product use	Did you consider reducing the emission of greenhouse gases when designing the use of your innovative product?
	Energy consumption from product use	Did you consider reducing energy consumption when designing the use of your innovative product?
	Emissions to water from product use	Did you consider reducing the emission to water when designing the use of your innovative product?

Aspects	Indicators	Questions
	Emissions to air from product use	Did you consider reducing the emission to air when designing the use of your innovative product?
	Waste production from product use	Are you in the process of reducing the waste generated during the product use?
	Less waste, less use of plastic in product use	Are you in the process of reducing the amount of packaging?
	Use of bio-based materials	Can you use bio-based packaging?
	Repairability of product	Can the product be easily repairable?
	Reuse of chemical substances in product	Can the product be easily reused?
	Recyclability: use of recycled raw materials and production of a recyclable innovative product	Can the product be recycled after use? Can the product be dismantled and separated to allow recycling of aspects of the product?
Economic sustainability	Direct benefits of use of product	Are there any direct economic benefits in using the innovative product?
Functionality	Durability	Is the MCNM* designed to have improved durability (the ability to remain functional)?
	Performance	Is the MCNM* designed to have improved performance (the action or process of performing a task or function)?
		Is the MCNM* designed to have an improved incorporating process (easier interaction with matrix, easier applicability, easier processing)?
	Reliability	Is the MCNM* designed to have an improved reliability (the quality of performing consistently well)?
	Useability	Is the MCNM* designed to have an improved useability (the quality or state of being usable)?
	Versatility	Is the MCNM* designed to be versatile (the quality to be used for different purposes)?
	Customer needs	Have customer needs been mapped?
	Target customer	Did you identify the target customer for the MCNM*?
	Process scalability	Can the design process phase be easily upscaled?
		Can the incorporating process phase be easily upscaled?
	Durability	Is the product incorporating the MCNM* designed to have an improved durability (the ability to remain functional)?
		Do you expect that the MCNM *could be modified during the USE phase (dissolution, release, agglomeration, surface reactivity)?

Aspects	Indicators	Questions
		Do you expect that the MCNM* surface modifications could affect functionality?
	Performance	Is the product incorporating the MCNM* designed to have an improved performance (the action or process of performing a task or function)?
	Reliability	Is the product incorporating the MCNM* designed to have an improved reliability (the quality of performing consistently well)?
	Useability	Is the product incorporating the MCNM* designed to have an improved useability (the quality or state of being usable)?
	Versatility	Is the product incorporating the MCNM* versatile (the quality to be used for different purposes)?
	Customer needs	Have customer needs been mapped?
	Target customer	Did you identify the target customer for the product MCNM*?
	Service issues	Can you identify any service issues (e.g., lower performances of the product) related to the product incorporating the MCNM*?

** As the questionnaire is of a comparative nature, the term MCNM is considered when assessing the MCNM. The term MCNM is replaced by the term benchmark when the benchmark is assessed*

2.2.5. End of Life treatment

This section shows how the end-of-life stage of the product incorporating the MCNM is addressed and considered within Tier 1. As reported in Table 5, there are four questions in this section, two for the first group (safety) and two for the second group (social and economic sustainability).

Table 5 Aspects, Indicators and Questions related to the End-of-Life stage.

Aspects	Indicators	Questions
Safety	Worker's exposition	Are workers exposed to MCNM* (i.e., via inhalation)?
	MCNM emission	Are there any expected MCNM *emissions into the environment?
Social sustainability	End-of-life information	Is there clear guidance on the end-of-life options provided through labelling?
Economic sustainability	Direct costs of end-of-life	Can you estimate the costs for the end-of-life scenarios of the innovative product?

** As the questionnaire is of a comparative nature, the term MCNM is considered when assessing the MCNM. The term MCNM is replaced by the term benchmark when the benchmark is assessed*

2.2.6. Comparison between SUNSHINE SSbD approach and Early4AdMa approach

The need for simplified methods that can be applied during the early stage of product development to identify safety and sustainability concerns related to advanced materials has attracted the attention of various research groups across Europe. In parallel with the developments within Sunshine, the Early Awareness and Action System for Advanced Materials (Early4AdMa) approach was simultaneously developed by the OECD. This early warning system is intended for regulators and policymakers to address safety, sustainability and regulatory issues, thereby supporting regulatory preparedness (OECD, 2023).

The Early4AdMa system presents a systematic approach designed to identify and address potential safety, sustainability, and regulatory issues associated with advanced materials in their early stages of development or use. It outlines that throughout the life cycle, the physical-chemical form of the advanced material may change through multiple transformation pathways, which need to be taken into account (OECD, 2023). The Early4AdMa leads to the identification

of appropriate follow-up actions when issues are detected. It aims to enhance regulatory preparedness by enabling policymakers, decision-makers, and regulators to proactively anticipate safety and sustainability challenges from emerging AdMa. Finally, it serves as a tool for anticipatory risk governance, fostering the safe and sustainable development of advanced materials while promoting innovation. The approach consists of two tiers. Tier 1 serves as a broad screening assessment, documenting advancements in AdMa and conducting a preliminary check for possible issues. Tier 1 consists of three steps. Step 1 involves scanning the field and selecting of an AdMa to assess. Step 2 conducts a screening assessment of health and environmental risks, sustainability, and regulatory issues by experts. Once a potential issue is identified during the initial assessment, Step 3 involves evaluating and describing the identified concerns. These steps are outlined in the (OECD, 2023) work, which provides a detailed, step-by-step guide on how to implement them. Tier 1 is optional, allowing users to bypass it if a potential issue with a specific material is already known.

Tier 2 involves answering four sets of questions and provides recommendations for follow-up actions such as further research or regulatory measures. These recommendations can be communicated to regulatory decision-makers to address potential issues at an early stage. Tier 2 is made up of four steps (Step 4,5,6,7). Step 4 consists of collecting additional information and context, focusing on gathering relevant information and contextual details related to the advanced material under evaluation, including benefits and socio-economic considerations. In Step 5, experts conduct a comprehensive analysis in various areas, including (1) Safety Assessment related to Human Health, evaluating the potential impact of the material on human health and well-being, (2) Safety Assessment for the Environment, evaluating the potential environmental consequences and risks associated with the material, (3) Applicability of Regulatory Frameworks, determining how existing regulatory frameworks apply to the material, identifying any gaps or considerations, and (4) Sustainability analysis, examining the material's sustainability aspects, such as resource usage, life cycle analysis, and environmental footprint. Then, Step 6 consists of the evaluation of the results from Step 5 and proposing potential follow-

up actions. Finally, Step 7 consists of monitoring both the assessment's impact and the follow-up actions.

Therefore, to identify similarities, possible overlaps and complementarities between these two similar approaches, and potential synergies for application by different stakeholders, a comparative analysis was performed. The comparison results can assist decision-makers in industry, policy, and regulation in selecting the most suitable methodology for their needs and guide follow-up actions. Accordingly, a comparison was made between Tier 1 of the SSbD approach developed in SUNSHINE and Tier 2 of Early4AdMa. Since both are SSbD approaches, they will be referred to as SUNSHINE Tier 1 (ST1) and Early4AdMa Tier 2 (ET2) in the following paragraphs for better differentiation.

The comparative analysis is illustrated in a case study, detailed in Chapter 1.3, a nanocomposite of graphene oxide functionalized with chitosan for use as a substitute for classical flame retardants. In the next paragraphs, the methodology adopted for the comparison between ST1 and ET2 is described.

To proceed with the comparison between the two approaches, the two sets of questions of ST1 and ET2 were classified in common aspect categories such as Safety, Environmental, Economic and Social sustainability, Functionality and Applicability to Regulatory Frameworks. Detailed Economic and Social sustainability aspects are specific only to the ST1, although these are generally considered in the context section of Early4AdMa (step 4). The Applicability to Regulatory Frameworks aspect is specific only to ET2. Once all the questions had been categorised within each aspect category, an assessment was conducted by reciprocally comparing the questions of one approach to the questions of the other. The similarities and differences between the questions were marked by colour-coding the questions. Green was used for equal questions, orange for questions that cover the same topic but are different, and red for questions that were considered only in one of the two approaches (Figure 3). A question from ST1 (or ET2) questionnaire was considered to be "equal" to one from ET2 (or ST1) if the answer to this question definitely provides the information required to respond to the corresponding ET2 (or ST1)

question (green label). If a question differs between both approaches but deals with the same theme, it is considered to have the “same topic” as another question (orange label). Lastly, if two questions do not share a common topic, the question is labelled as "not considered" in the other approach’s questionnaire (red label).

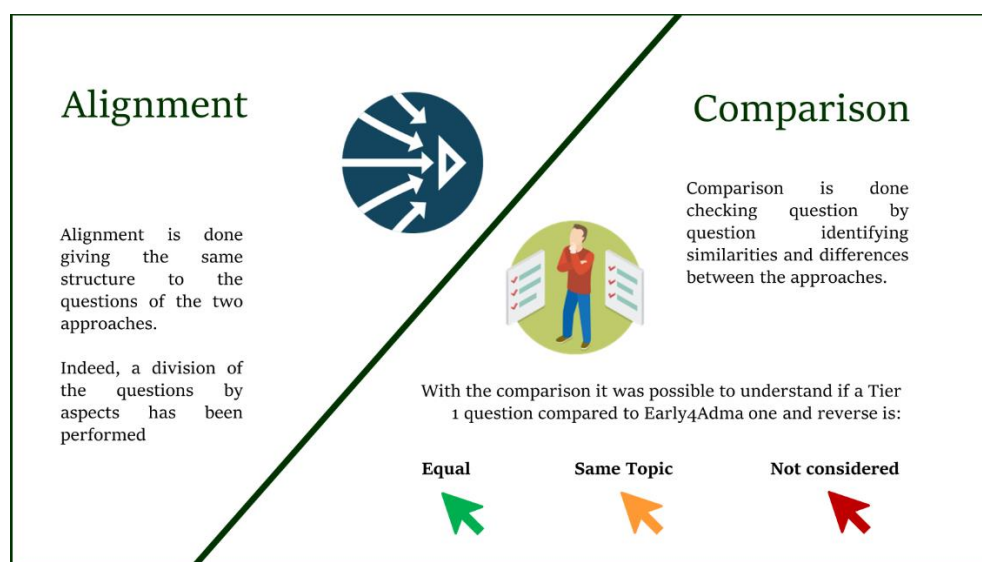


Figure 3 Method for alignment and comparison between SUNSHINE Tier 1 (ST1) and Early4AdMa Tier 2 (ET2).

The ST1 and ET2 questionnaires were submitted to a company that produces an innovative flame retardant described in Chapter 1.3. Thanks to the application of ET2 and ST1 to the selected case study, it was possible to compare the outcomes derived from the implementation of both methods and confirm the results of the comparison. The outcomes of the comparison are reported in Chapter 3.1.1.

2.3.Tier 2

Tier 2 consists of the REACH Chemical Safety Assessment (CSA) approach and Life Cycle Sustainability Assessment (LCSA) methodologies, in line with the SSbD Framework proposed by the JRC. While in Tier 1, aspects related to safety have been included in the assessment and applied to case studies, a full regulatory CSA is out of the scope of this thesis, since it has been performed in SUNSHINE by partners with a strong background in occupational and consumer risk assessment. The focus of this thesis is indeed on Life Cycle Assessment (LCA), Life Cycle Costing

(LCC) and Social Life Cycle Assessment (S-LCA). When conducting an LCA, LCC or S-LCA, all life cycle stages of the product being studied are mapped, including raw materials acquisition, manufacturing, as well as use and End-of-Life (EoL) management, from cradle to grave (Jolliet et al., 2015). Life Cycle Sustainability Assessment methodologies are not described in the following chapter, as they have already been thoroughly presented in Chapter 1.2 "State of the Art of the Life Cycle Sustainability Assessment". However, a description of the software tools used to implement LCSA methodologies is provided below.

LCA methodology can be conducted using software such as OpenLCA (<https://www.openlca.org/>) or SimaPro (<https://simapro.com/life-cycle-assessment/>). SimaPro was chosen due to its status as the most widely utilized LCA software, offering significant flexibility and a wide array of features. This professional tool is designed to collect, analyze, and monitor sustainability performance data for a company's products and services. SimaPro supports various applications, including sustainability reporting, carbon and water footprints, product design, generating environmental product declarations, and determining key performance indicators. Additionally, it incorporates the most recent version of the leading life cycle inventory data source, Ecoinvent Version 3 (Wernet et al., 2016). The Ecoinvent database contains comprehensive international industrial life cycle inventory data, covering energy supply, resource extraction, material supply, chemicals, metals, agriculture, waste management services, and transport services. It adheres to ISO 14040 and 14044 standards for LCA studies and assessments, ensuring transparency and consistency. Each dataset is provided as a unit process and an aggregated system process.

To conduct an LCC analysis, software as D-LCC, One Click LCA, or SimaPro can be used. The software SimaPro can be used by creating a tailored method. To achieve this, a set of cost categories needs to be specified, and a conversion factor must be specified for each one. For instance, the cost per kWh for the different energy sources of the cost category "Energy" needs to be specified. Once the conversion factor is established for each cost sub-category, the costs can be aggregated based on the amount of a specific process (e.g., energy) used.

To conduct a S-LCA, the SimaPro software can be used, importing a database as the Social Hotspot Database (SHDB). The assessment described in this thesis was conducted using the Social Hotspots Database (SHDB). The SHDB encompasses data on supply chain composition, labour intensity, and social risk information. Supply chains are geographically specific and generated through the Global Trade Analysis Project (GTAP) model. Data is organized by country, with each country having a list of relevant sectors identified using the GTAP model. The country/sector data is expressed in worker hours, serving as an activity variable that indicates the location and intensity of human activity within the supply chain. Although the activity variable is explicitly linked to the worker stakeholder category, it is considered the most effective means of assessing the scale of social issues for all stakeholder categories throughout the supply chain (Norris et al., 2019)

3. Chapter 3 Results

This chapter presents the results of applying SUNSHINE SSbD approach Tier 1 to the selected case studies (3.1), comparing SUNSHINE Tier 1 and Early4AdMa Tier 2 (3.1.1), and applying SUNSHINE Tier 2 to the selected case studies (3.2).

3.1. Tier 1 results for anti-sticking coating, active food packaging, and ACRE TFT case studies

As reported in Chapter 2.2, Tier 1 consists of four parts, where the first part is the introduction to the questionnaire, the second and third parts are general questions to get familiar with the case study and have not applied in the SUNSHINE project, while the fourth part includes the set of detailed questions applicable during the R&D stage which is the focus of this thesis. The possible answers to each question belonging to the fourth part are “Yes”, “No”, “I don’t know” and “Not applicable”. The assessment is performed by comparing either the material/product against a benchmark (i.e., another existing material/product which has the same function) or comparing alternative modification options (e.g., different coatings).

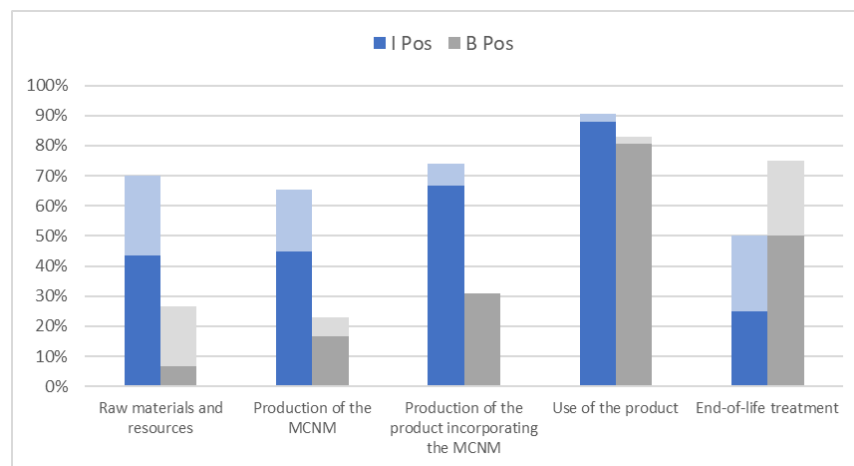
The Excel sheet containing the questions filled by the case studies and the responses, is included in Annex 3.

In the following paragraphs, the results of the application of the questionnaire to the anti-sticking coating case study, the active food packaging case study and the ACRE TFT case study are reported. The results of the questionnaires related to the anti-sticking coating case study are shown in Figure 4, Figure 5 and Figure 6, and those related to the active food packaging are shown in Figure 7, Figure 8 and Figure 9.

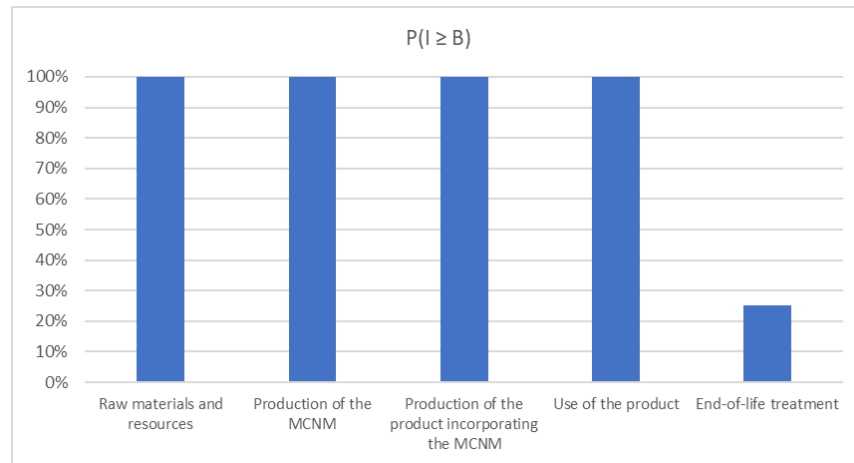
The blue columns report the results for the innovative material, while the grey ones those for the benchmark. The light blue and light grey parts of the column show the relative uncertainty for both the innovative MCNM and the benchmark. This implies that when the actual positives plus the uncertainty of an alternative (i.e. the total height of a column) is below of the actual positives only of another alternative (i.e. the dark colour part only), then, the probability of the latter being

better than the former is 100% as even if all the former's uncertain answers would turn into positives they will not ever be higher than the latter.

Specifically, Figure 4a and Figure 7a show the percentage of positive contributions for the innovative material and the benchmark by life cycle stages (Raw materials and resources needed to produce the material/product, Production of the MCNM, Production of the product incorporating the MCNM, Use of the product, and End of life treatment) and Figure 4b and Figure 7b show the probability on the y-axis, for each life cycle stage, that the innovative MCNM is better or equal than the benchmark. In addition, Figure 5a and Figure 8a show the percentage of positive contributions for the two assessed materials divided on the basis of the safety, environmental, social and economic sustainability and functionality aspects, while Figure 5b and Figure 8b shows the probability on the y-axis, for each aspect, that the innovative MCNM is better or equal than the benchmark. Finally, Figure 6a and Figure 9a show the overall percentage of positive contributions for the innovative material and the benchmark, while Figure 6b and Figure 9b show the overall probability on the y-axis that the innovative MCNM is better or equal than the benchmark.

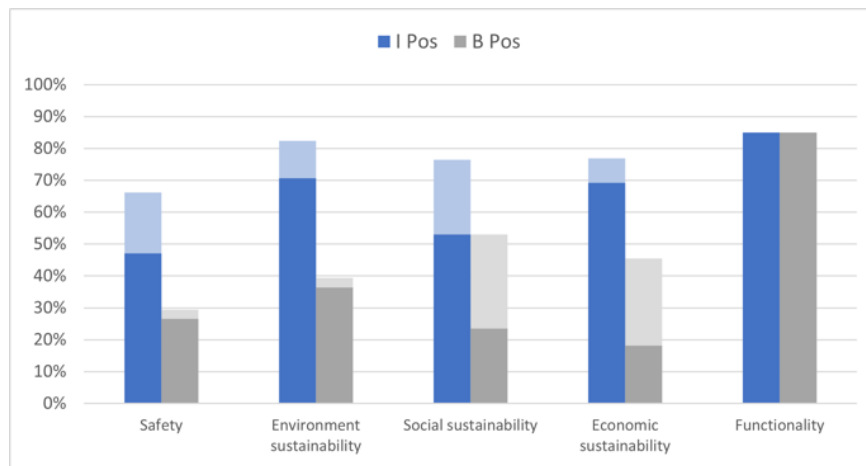


a

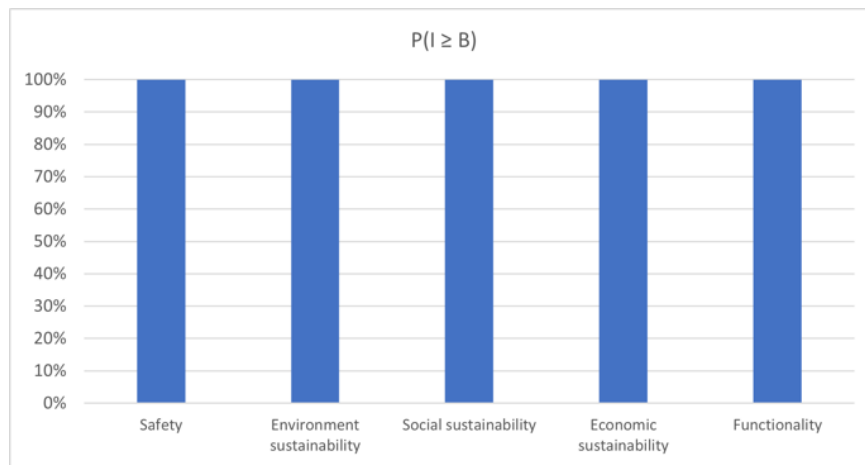


b

Figure 4 Anti-sticking coating case study (a) Percentage of positive contributions by life cycle stages; (b) Probability that the innovative MCNM is better or equal than the benchmark for each life cycle stages. I Pos = positive contributions for the Innovative material; B Pos = positive contributions for the benchmark. Life cycle stages: Raw materials and resources needed to produce the material/product, Production of the MCNM, Production of the product incorporating the MCNM, Use of the product, and End-of-life treatment. The light blue and light grey parts of the column show the relative uncertainty for both the innovative MCNM and the benchmark.

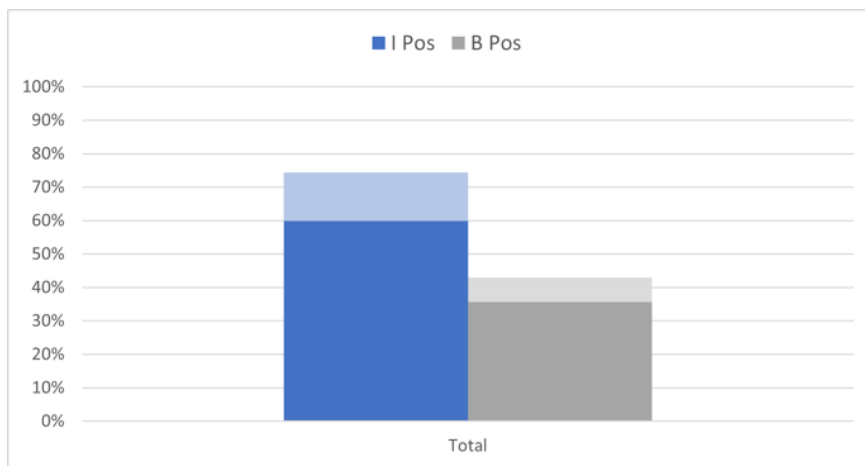


a

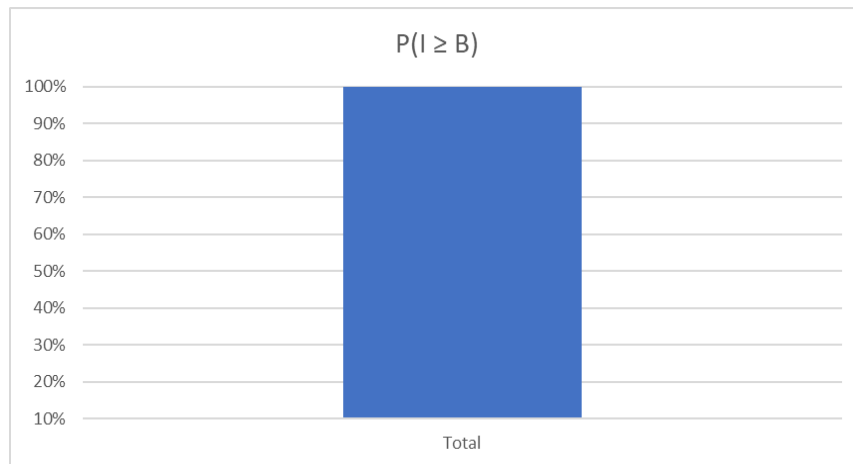


b

Figure 5 Anti-sticking coating case study (a) Percentage of positive contributions by aspects; (b) Probability that the innovative MCNM is better or equal to the benchmark for each aspect. The light blue and light grey parts of the column show the relative uncertainty for both the innovative MCNM and the benchmark.



a



b

Figure 6 Anti-sticking coating case study (a) Total percentage of positive contributions for the innovative material and the benchmark; (b) Probability that the innovative MCNM is better or equal than the benchmark. The light blue and light grey parts of the column show the relative uncertainty for both the innovative MCNM and the benchmark.

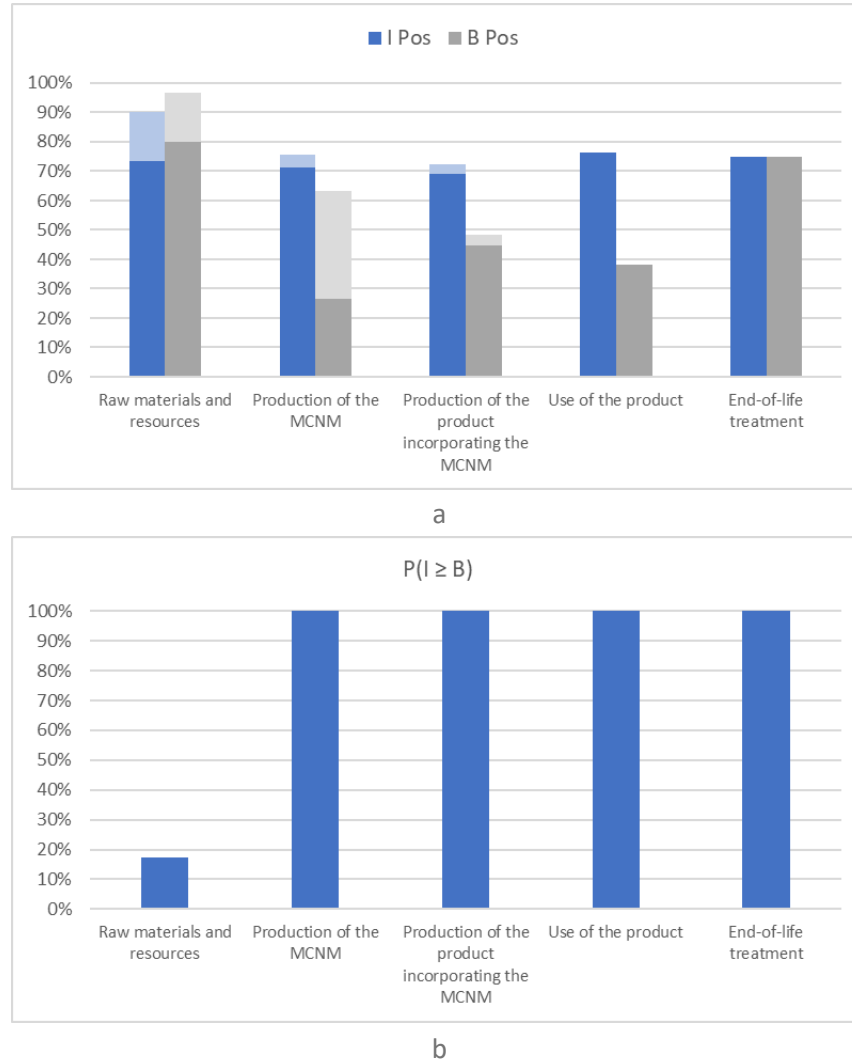
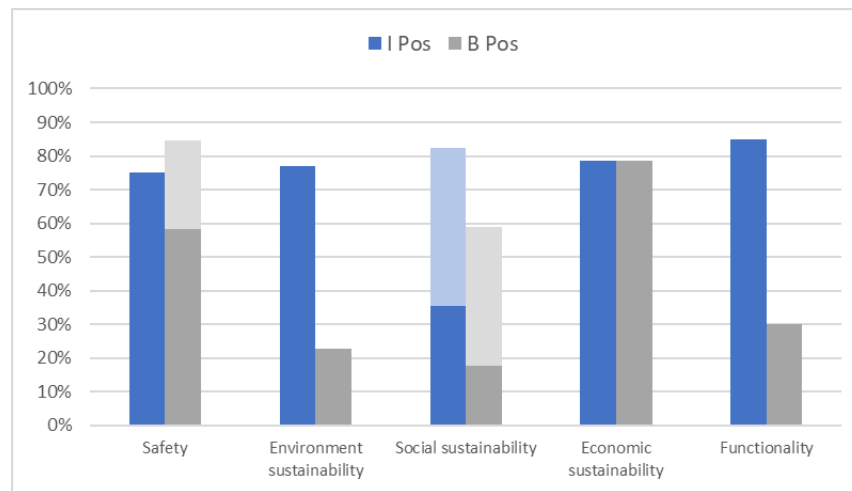
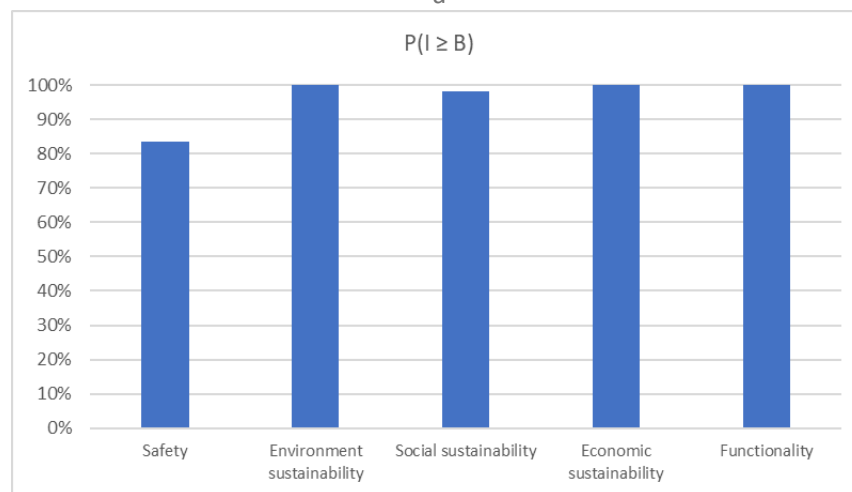


Figure 7 Active food packaging case study (a) Percentage of positive contributions by life cycle stages; (b) Probability that the innovative MCNM is better or equal than the benchmark for each life cycle stages. I Pos = positive contributions for the Innovative material; B Pos = positive contributions for the benchmark. Life cycle stages: Raw materials and resources needed to produce the material/product, Production of the MCNM, Production of the product incorporating the MCNM, Use of the product, and End-of-life treatment. The light blue and light grey parts of the column show the relative uncertainty for both the innovative MCNM and the benchmark.

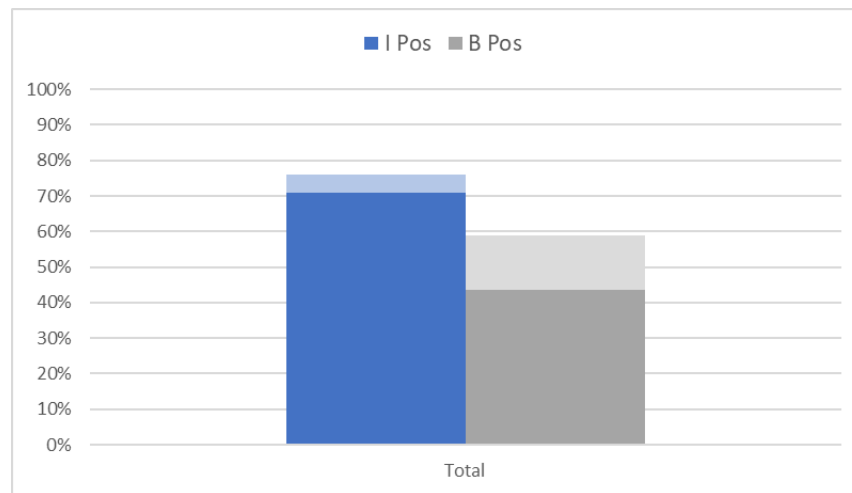


a

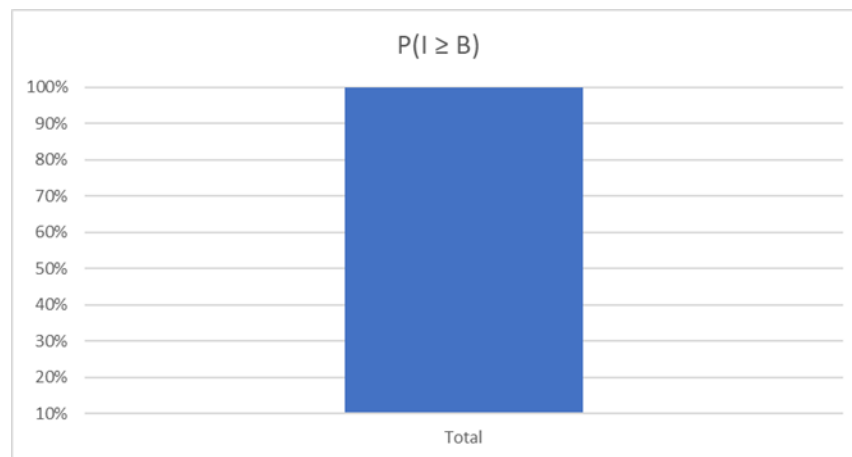


b

Figure 8 Active food packaging case study (a) Percentage of positive contributions by aspects; (b) Probability that the innovative MCNM is better or equal than the benchmark for each aspect. The light blue and light grey parts of the column show the relative uncertainty for both the innovative MCNM and the benchmark.



a



b

Figure 9 Active food packaging case study(a) Total percentage of positive contributions for the innovative material and the benchmark; (b) Probability that the innovative MCNM is better or equal than the benchmark. The light blue and light grey parts of the column show the relative uncertainty for both the innovative MCNM and the benchmark.

The application of the questionnaire to the ACRE TFT case study was not straightforward due to limited available data. Specifically, there was no benchmark information accessible from those who filled the questionnaire. As for the ACRE TFT, the information provided was quite minimal. For every life cycle stage except for raw materials, the responses to the questionnaire were uniformly "I don't know," reflecting a significant gap in the available data. In the case of the raw materials stage, responses were given for only 7 out of the 31 questions, indicating a similar lack of comprehensive information. This happened because the product being developed is still in a very early stage of development. Since the availability of information is crucial for the successful

implementation of the questionnaire, this attempt provided an opportunity to assess when the questionnaire can effectively be applied and when it cannot. The results obtained from the application of the Tier 1 questionnaire to the case studies are discussed in Chapter 4.1.

3.1.1. Comparison between SUNSHINE SSbD approach and Early4AdMa approach

Following the methodology provided in Chapter 2.2.6, a comparative analysis between SUNSHINE Tier 1 (ST1) and Early4AdMa Tier 2 (ET2) questions was carried out. To indicate the level of similarity between the questions, the following colour scheme was employed: green for “equal”, orange for “same topic” and red for “not considered” questions. ST1 is composed of 154 questions, while ET2 has 65 questions. From Figure 10, it can be noted that ST1 has 26 questions that are equal, 69 that address the same topic and 59 that are not considered in ET2. On the other hand, ET2 has 16 equal questions, 26 that address the same topic and 23 that are not considered in ST1.

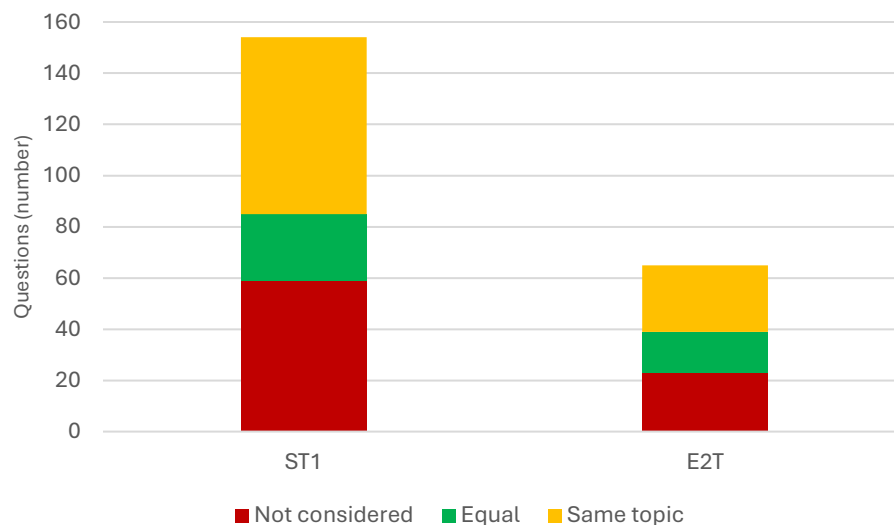


Figure 10 Number of questions that are the same, with a shared topic, or not present between SUNSHINE Tier 1 (ST1) and Early4AdMa Tier 2 (ET2).

The number of “equal” questions between the two approaches is not the same. The reason for this difference lies in the method used to compare the questions. As mentioned earlier, a question in the ST1 is considered “equal” to a question in the ET2, and vice versa, if the answer to a

question in the first provides the information to respond to the corresponding question in the second. During the comparison between the questions, it often happened that in one of the two approaches, a question was composed of more than one question from the other approach. For example, within ST1, there are two questions related to the Safety aspect, which ask respectively if the material is 1) carcinogenic and 2) genotoxic (mutagenic). Within ET2, there is a single question asking if there is an indication of carcinogenicity/genotoxicity/mutagenicity of the material. Therefore, the information collected from the single question of ET2 can be used to answer two questions of ST1. In this way, two questions of the ST1 are considered equal to one of ET2.

In addition, there is a disparity in the number of questions between the two approaches. ST1 comprises 154 questions, while ET2 has 65 questions. To ensure a fair comparison, the results were converted into percentages (Figure 11).

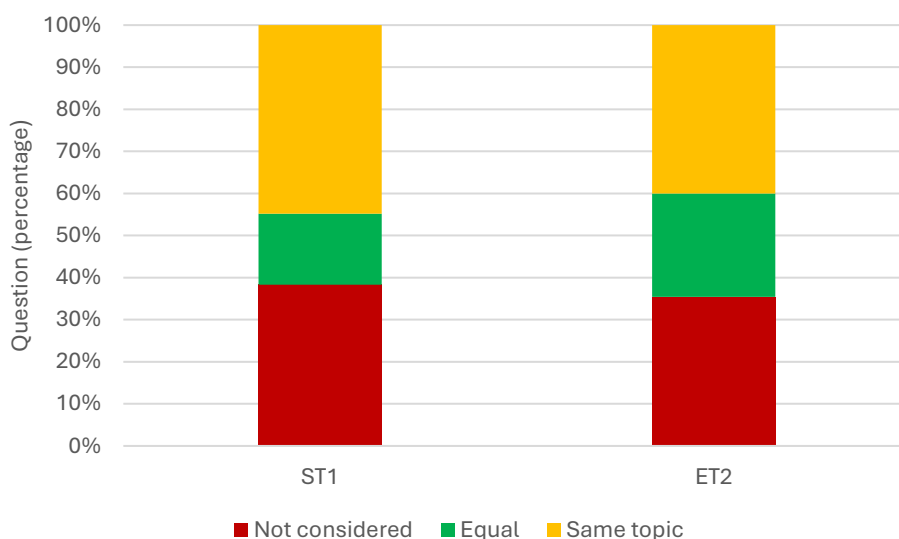


Figure 11 Percentage of questions that are the same, with a shared topic, or not present between SUNSHINE Tier 1 (ST1) and Early4AdMa Tier 2 (ET2).

From Figure 11, ST1 has 17% of questions that are equal, 38% that address the same topic and 45% that are not considered in ET2. On the other hand, ET2 has 25% questions that are equal, 45% that address the same topic and 38% that are not considered in ST1. The percentage of “not considered” questions is quite high, and it is because specific aspects are considered only by one

of the two approaches. Indeed, from Figure 12, it is possible to observe which aspects are or are not covered by the two methodologies. Figure 12 shows that Safety and Environmental sustainability are addressed by both ST1 and ET2, while Social and Economic sustainability are specifically addressed by ST1. Additionally, Applicability to Regulatory Frameworks is only covered by ET2 while Functionality is only partly addressed by ET2. Indeed, Functionality is not addressed in ET2, however, related questions are included under other aspects.

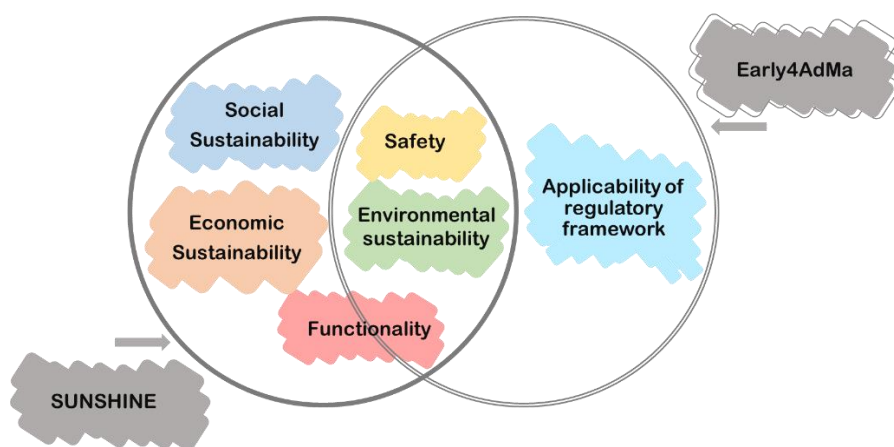


Figure 12 Aspects covered and partially covered by SUNSHINE and Early4AdMa approaches.

A detailed breakdown of the number of questions categorized as "equal," "same topic," and "not considered" for each aspect is shown in Figure 13. Specifically, regarding the Safety aspect, ST1 has 20 (29.4%) equal questions, 45 (66.2%) that share the same topic, and 3 (4.4%) that are not considered in ET2. On the other hand, ET2 has 12 (32%) equal questions, 15 (41%) that share the same topic, and 10 (27%) that are not considered in ST1. Then, regarding the Environmental sustainability aspect, ST1 has 4 (11%) equal questions, 25 (71%) that share the same topic, and 6 (17%) that are not considered in ET2. On the other hand, ET2 has 4 (25%) equal questions, 11 (69%) that share the same topic, and 1 (6%) that is not considered in ST1. Concerning the Social sustainability, Economic sustainability, and Functionality aspects, ST1 has 17, 13, and 20 questions respectively (100%) that are not considered in ET2. Indeed, these aspects are not addressed in ET2. This is clearly illustrated in Figure 13, where the column representing the number of questions categorized as equal, same topic, and not considered for ET2 regarding these topics is

shown to be at 0. Finally, regarding the Applicability to the Regulatory Framework aspect, ET2 has 12 (100%) questions that are not considered in ST1. This is clearly illustrated in Figure 13, where the column representing the number of questions categorized as equal, same topic, and not considered for ST1 regarding this topic is shown to be at 0

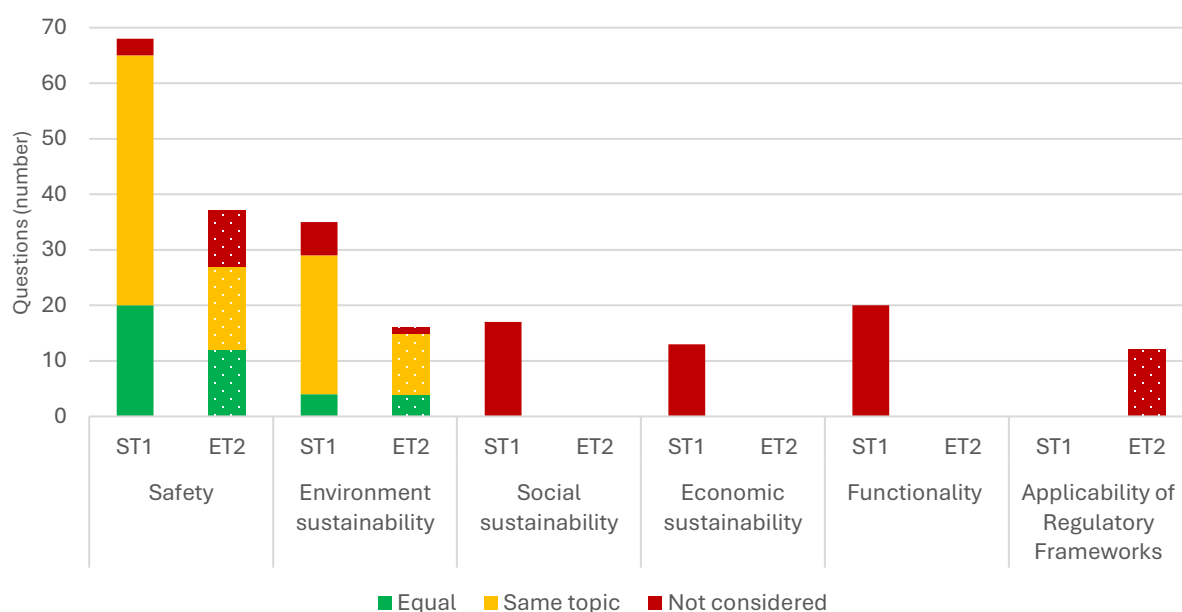


Figure 13 Number of questions categorized as "equal", "same topic," and "not considered" for each aspect of SUNSHINE Tier 1 (ST1) and Early4AdMa Tier 2 (ET2). The histograms representing ST1 results are shown in full color, while those for ET2 are marked with white dots

The comparison between ST1 and ET2 allowed the identification of similarities, differences and complementarities, which are reported in Table 6 and discussed in Chapter 4.1.1

Table 6 Similarities, differences and complementarities identified comparing ST1 and ET2.

	ST 1	ET2
Aspects	Safety, Environmental, Social and Economic sustainability and Functionality	Safety, Environmental Sustainability, and Applicability to Regulatory Framework
Aims	To support industries, especially SMEs, in identifying safety and sustainability hotspots of concern, as well as in comparing SSbD design alternatives in the early stages of innovation	To support regulators in increasing regulatory preparedness, but also companies in anticipating incoming changes to regulations and the related guidance

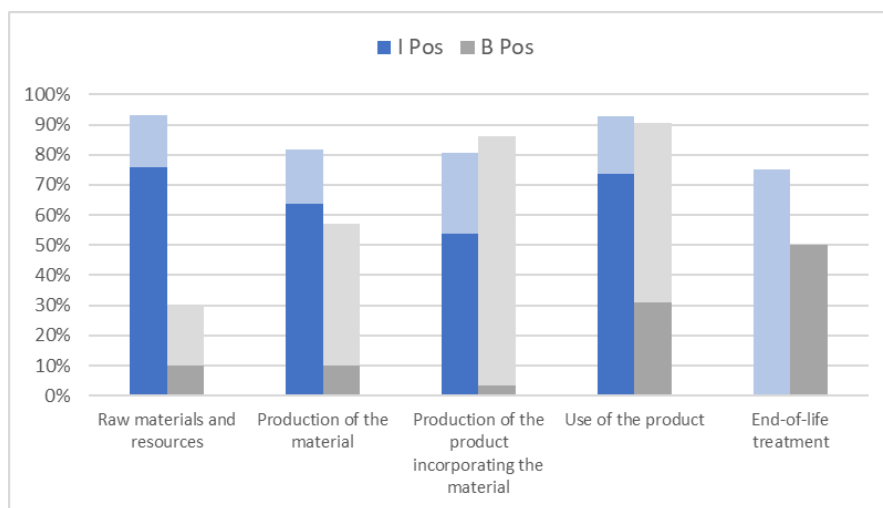
User groups	Self-assessment methodology targeted at industries, especially SMEs	Early warning system targeted at policymakers and regulators
Comparability	Comparative	Not comparative
Division of the questions	By life cycle stages (LCS), where for each LCS, the questions are divided by aspects	By aspects
Results	1) Showed according to aspects, LCS and as an overall performance 2) Showed as a potential positive contribution	1) Showed according to aspects 2) Showed as potential avoided issues
Uncertainty	Calculated using the “I don’t know” answers	Not assessed

ST1 applied to innovative flame retardant case study

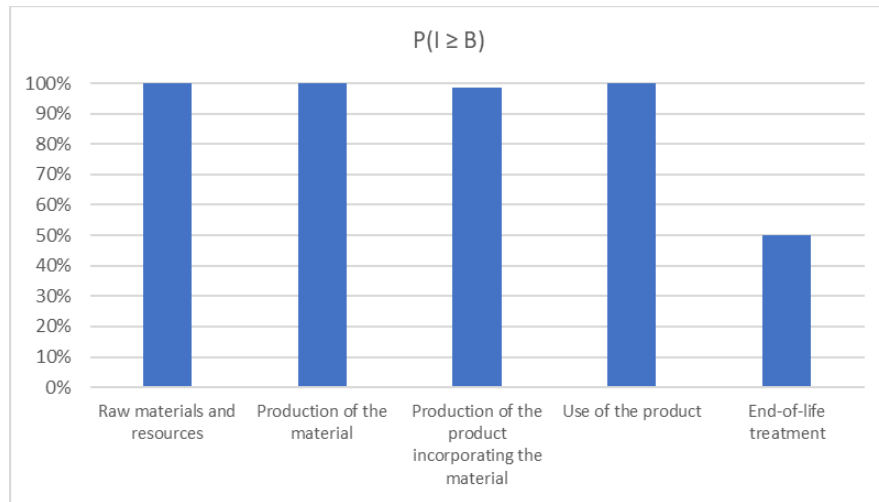
Since ST1 involves a comparative analysis, the innovative flame retardant was compared to a benchmark, i.e., melamine cyanuric acid, which is a classical flame retardant. The results of this comparison can be seen in Figure 14, Figure 15 and Figure 16. The blue columns report the results for the innovative material, while the grey ones are those for the benchmark. The light blue and light grey parts of the column show the relative uncertainty for both the innovative material and the benchmark.

Specifically, Figure 14a shows the percentage of positive contributions by life cycle stages and Figure 14b shows the probability on the y-axis, for each life cycle stage, that the innovative material is better or equal to the benchmark. In addition, Figure 15a shows the percentage of positive contributions based on the Safety, Environmental, Social and Economic sustainability and Functionality aspects, while Figure 15b shows the probability on the y-axis, for each aspect, that the innovative material is better or equal to the benchmark. Finally, Figure 16a shows the overall percentage of positive contributions for the innovative material and the benchmark, while Figure 16b shows the overall probability on the y-axis that the innovative material is better or equal to the benchmark.

Figure 14a shows that the innovative flame retardant performs better when considering the overall percentage of positive contributions than the melamine cyanuric acid for all five assessed life cycle stages. However, it must be considered that the uncertainty is very high, given that many questions in the questionnaire were answered with "I don't know". Also, the probability that the innovative coating material is better or equal to the benchmark for each life cycle stage is almost 100% for four LCS (Life Cycle Stages) and 50% for the last, the End-of-life treatment (Figure 14b).



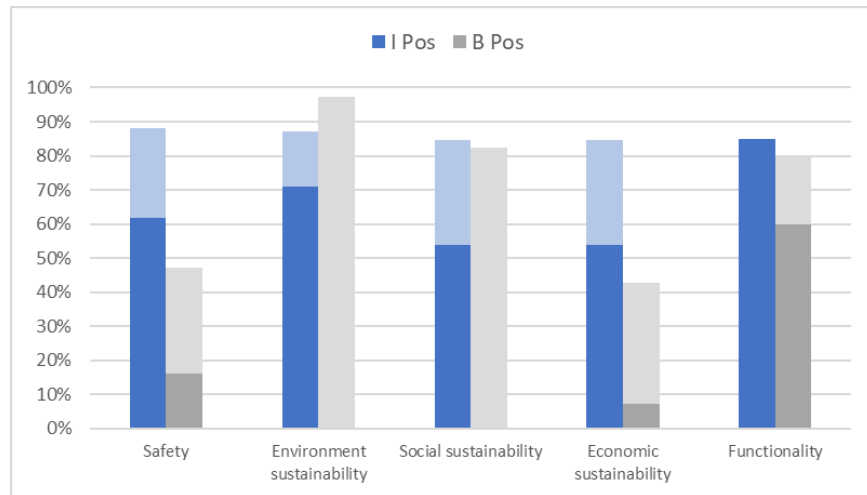
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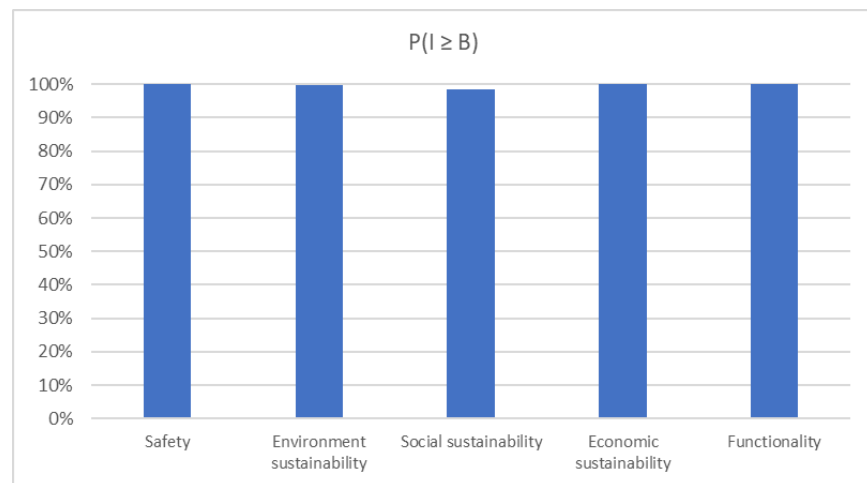
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Figure 14 Innovative flame retardant case study (a) Percentage of positive contributions by life cycle stages; (b) Probability that the innovative material is better or equal than the benchmark for each life cycle stages. I Pos = positive contributions for the Innovative material; B Pos = positive contributions for the benchmark. Life cycle stages: Raw materials and resources needed to produce the material/product, Production of the advanced material, Production of the product incorporating the advanced material, Use of the product, and End-of-life treatment. The light blue and light grey parts of the column show the relative uncertainty for both the innovative material and the benchmark.

The percentage of positive contributions, as previously reported for the life cycle stages, has also been estimated for Economic, Environmental and Social sustainability, Safety and Functionality aspects (Figure 15). Specifically, Figure 15a shows that the innovative flame retardant performs better in all these aspects. However, for almost all aspects, the related uncertainty is quite high. Figure 15b shows the probability that the innovative flame retardant is better or equal to the benchmark for each aspect, which is 100% for all the LCS except for Social sustainability, which is 98%.



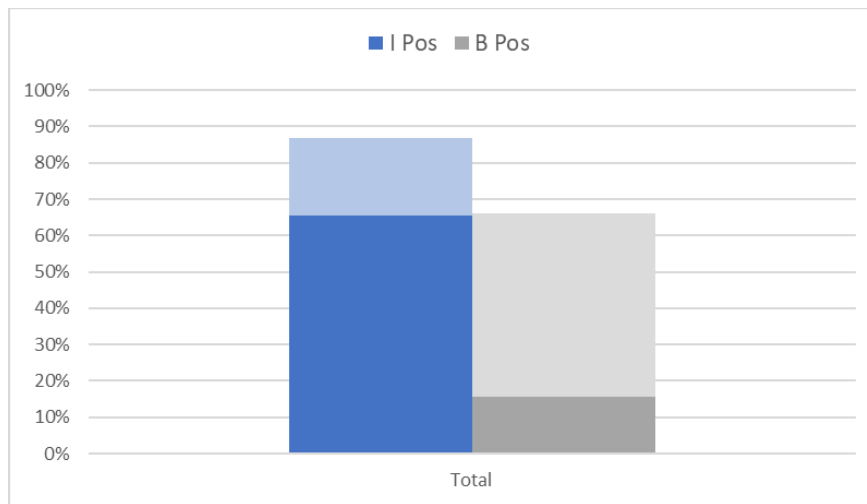
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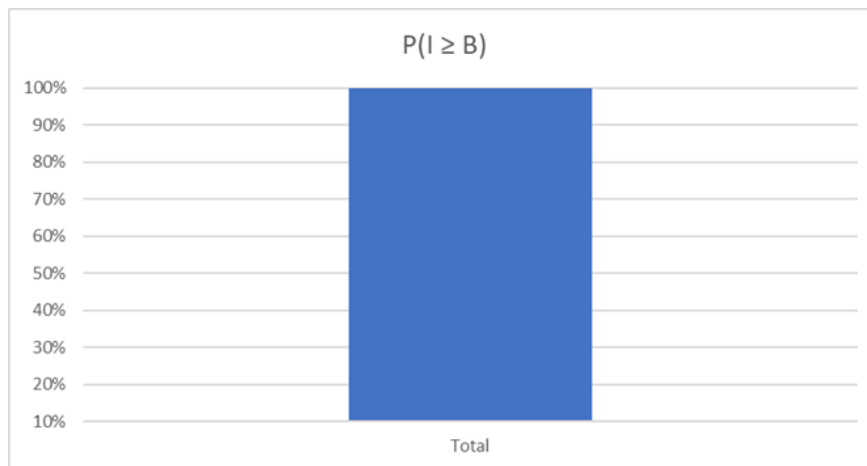
b

Figure 15 Innovative flame retardant case study (a) Percentage of positive contributions by aspects; (b) Probability that the innovative material is better or equal than the benchmark for each aspect. The light blue and light grey parts of the column show the relative uncertainty for both the innovative material and the benchmark.

In Figure 16a, all positive contributions related to the two compared alternatives are shown. Figure 16a demonstrates that the innovative material has a higher percentage of positive contributions than the benchmark, while Figure 16b shows that the overall probability that the innovative material is better or equal than the benchmark is 100%.



a



b

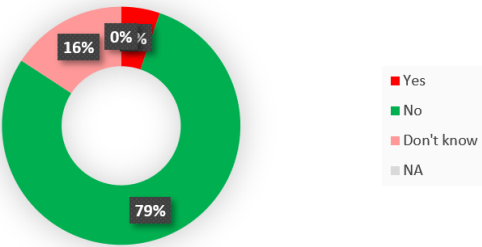
Figure 16 Innovative flame retardant case study (a) Total percentage of positive contributions for the innovative material and the benchmark; (b) Probability that the innovative material is better or equal than the benchmark. The light blue and light grey parts of the column show the relative uncertainty for both the innovative material and the benchmark.

ET2 applied to innovative flame retardant case study

The ET2 questionnaire was applied to the innovative flame retardant, one of the SUNSHINE project's case studies. The company that produces the product provided the answers to ET2 questions related to the innovative flame retardant, which are graphically represented in Figure 17. In ET2, questions are structured in a way that the "Yes" response points to a potential issue

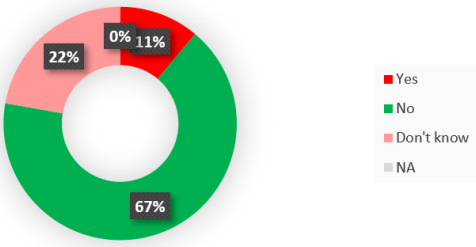
identified. As a result, the red section in the donut charts (Figure 17) represents the percentage of potential issues about a specific aspect. The green section indicates the percentage of potential issues that are not expected, the pink section represents the percentage of information gaps, and the grey section represents the percentage of unanswered questions due to their inapplicability.

Safety assessment - Human Health



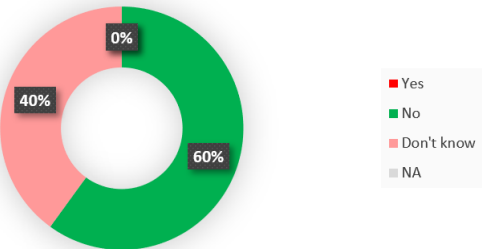
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Safety assessment - Environment



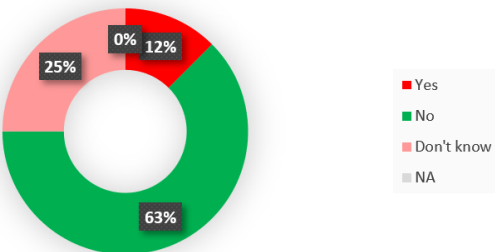
b

Applicability of Regulatory Frameworks



c

Sustainability



d

Figure 17 Innovative flame retardant results as percentage of potential issue (Yes) potential avoided issues (No) knowledge gaps (Don't know), not applicability of the question (NA).

Figure 17a shows that the innovative flame retardant results in a 5% potential human health safety issues, while 79% of the answers point out that the related issues have been avoided. Additionally, there is a 16% information gap related to the fact that the company is not able to provide the requested information. Figure 17b shows that the innovative flame retardant results in 11% potential environmental safety issues, while 67% of the answers point out that the related issues have been avoided. Additionally, there is a 22% information gap. Figure 17c shows that the innovative flame retardant results in 60% of answers, which points out that the Applicability to

Regulatory Frameworks issues have been largely avoided, but there is still a 40% information gap. Finally, Figure 17d shows that the innovative flame-retardant results in 12% potential environmental sustainability issues, while 63% of the answers point out that the related issues have been avoided. Additionally, there is a 25% information gap.

Validation of ST1 and ET2 comparison

The results obtained from the applications of the two approaches to the innovative flame retardant, as displayed in Figure 14, Figure 15, Figure 16, and Figure 17 are presented in different formats. This necessitates a thorough validation process to compare the findings. Indeed, the responses to questions deemed equal or about the same topic across the different approaches were examined. This allowed to determine if the questions considered equal between the two approaches are indeed the same, and if it is possible to compare responses to questions with similar topics. Table 7 displays the number of responses that are identical (N° =), different (N° X), or not evaluable (N° n.e.) for those questions of ST1 (or ET2) considered equivalent or with the topic shared to those of ET2 (or ST1). Some responses were considered not evaluable (n.e.) because a question in one questionnaire had multiple corresponding questions in the other. The related percentages were then calculated based on the total number of responses (Table 7). In ST1, out of 26 questions deemed equivalent to ET2, 13 responses were the same, and 13 were different (Table 7). The different responses were likely due to the ST1 questionnaire being completed before the ET2 questionnaire, leading to changes in responses from "I don't know" to "yes" or "no". Furthermore, out of 69 questions with a shared topic between ST1 and ET2, 6 responses were the same, 38 were different, and 25 were not assessable. Upon examination of the data, it is evident that among 26 questions identified as equivalent to ET2, 50% of responses matched, while the remaining 50% varied (Table 7). Additionally, of the 69 questions related to shared topics between ST1 and ET2, 9% of responses aligned, 55% differed, and 36% could not be assessed. For ET2, out of 16 questions deemed equivalent to ST1, 10 responses were the same, and 6 were different. Additionally, out of 26 questions with a shared topic between ET2 and ST1, 3 responses were the same, 5 were different, and 18 were not assessable. After analyzing the data, it is evident that among 16 questions identified as equivalent to ET2, 63% of responses

matched, while the remaining 38% varied (Table 7). Additionally, of the 26 questions related to shared topics between ST1 and ET2, 12% of responses aligned, 19% differed, and 69 % could not be assessed. The results obtained from the comparison between ST1 and ST2 are discussed in Chapter 4.1.1,

Table 7: Number and percentage of responses that are identical ((N° =) (% =)), different ((N° X) (% X)), or not evaluable ((N° n.e.) (% n.e.)) for questions considered equivalent or that shared a topic between ST1 and ET2.

Approach	Type	N° =	N° X	N° n.e.	Tot	% =	% X	% n.e.
<u>ST1</u>	<i>Equal</i>	13	13	0	26	50%	50%	0%
	<i>Same topic</i>	6	38	25	69	9%	55%	36%
<u>ET2</u>	<i>Equal</i>	10	6	0	16	63%	38%	0%
	<i>Same topic</i>	3	5	18	26	12%	19%	69%

3.2.Tier 2

In this chapter, the results of applying Life Cycle Sustainability Assessment (LCSA) methodologies to the anti-sticking coating (3.2.1), the active food packaging (3.2.2) and the ACRE TFT (3.2.3) case studies are presented. For each case study, the following sections are reported: Goal and scope definition, System boundaries, Life cycle inventory and Life Cycle Impact Assessment. For each section, information is reported both for the innovative products and the related benchmarks.

3.2.1.Anti-stick coating

3.2.1.1. Goal and scope definition

The goal of LCA, LCC and S-LCA was to minimise the environmental impacts of the anti-sticking coating, a MCNM made of silica carbide and titanium dioxide (SiC@TiO_2) to be applied to a baking tray described in Chapter 1.3, while optimising its social and economic cost-benefit ratio.

The functional unit (FU) selected was the coating of 1 m^2 of an industrial baking tray for five-year of its use. The baking tray is coated with either the MCNM or the benchmark material (i.e., a Teflon® based coating). In this time frame, the MCNM coating is re-applied twice a year on the baking tray after the removal of the old layer, while the tray coated with the benchmark is disposed wholly every year. In the study, the impacts of the use of the tray at high temperatures are not considered as well as the release of material in food is not assessed. Data for the benchmark derives from LCA database processes and literature review.

3.2.1.2. System boundaries

In the following paragraphs, the system boundaries of the anti-sticking coated baked tray and of the benchmark are described.

Anti-sticking coating

Based on information obtained from Laurentia company which produces the anti-sticking coating made of silica carbide and titanium dioxide (SiC@TiO_2), the coating was modelled within the software SimaPro. The diagram of the system under assessment is illustrated in Figure 18.

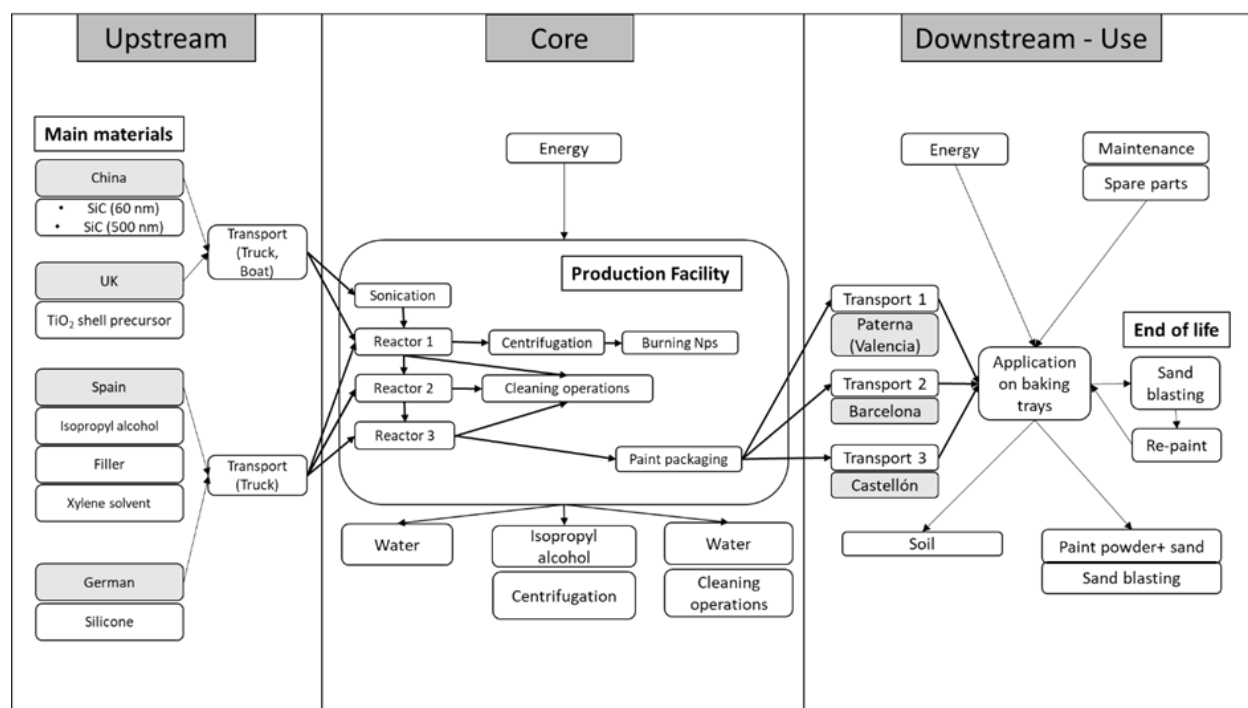


Figure 18 Upstream, Core and Downstream-Use of anti-sticking coated baking tray.

In the LCA study, energy and matter flows related to the Upstream, Core and Downstream stages of the anti-sticking coating applied to a baking tray are considered. As shown in Figure 18, the main materials are purchased from China, United Kingdom, Spain, and Germany. From these countries, the main materials are transported by truck and boat to Laurentia company, where the manufacturing core process of the SiC@TiO₂ takes place. Once this process is complete, the SiC@TiO₂ compound is shipped from Laurentia company to Valencia, Barcelona, and Castillon to be applied on a steel baking tray. The company was unable to ascertain the origin of the steel baking tray. Therefore, it was decided to select a baking tray with a global origin to ensure a more generalized and comprehensive scenario. Regarding the end-of-life, the baking tray coated with SiC@TiO₂, after six months of usage, is sandblasted and re-painted to be used again.

For the LCC and S-LCA, the costs related to Upstream (materials and their transportation), Core (electricity for the production processes, and treatment for the waste produced) and Downstream (baking tray maintenance, transport of the baking tray to the maintenance, electricity for the maintenance) stages were considered. The shipment costs to other countries

were not available and therefore were not included in the assessment. During the use stage, certain assumptions were made about the baking tray, including its origin and cost. Since the materials' origin significantly impacts the results of S-LCA (e.g., materials sourced from areas with poor labor practices or weak regulations may result in higher social risks, such as child labor and poor working conditions), three scenarios were considered to account for geographical diversities of the supply (Devecchi et al., In press). The first scenario involves a tray and coating process located in China. The second and third scenarios have these activities taking place respectively in the USA and Europe facility (Devecchi et al., In press). Regarding the Downstream stage, the end-of-life treatment of the baking tray was considered only for the LCC, since the S-LCA database (SHDB) still has no waste disposal process available.

Benchmark

Information about the benchmark was retrieved from the literature, which introduces certain limitations to the modelling of LCA, LCC, and S-LCA. For the LCA, the process was more straightforward as the Teflon® process is included within the Ecoinvent database. In contrast, the S-LCA faced challenges due to the absence of the Teflon® process in the Social Hotspots Database (SHDB). Additionally, the LCA considers the end-of-life phase of the product, whereas the S-LCA does not, as the SHDB currently lacks waste disposal processes.

For the LCA of the benchmark, the baking tray coated with Teflon®, data from the Ecoinvent database served as the primary reference. This included the Teflon® and the baking tray, as well as the energy required to apply the Teflon® to the baking tray. Regarding the end-of-life, the tray coated with the benchmark is recycled wholly every year. The diagram of the system under assessment according to the LCA is illustrated in Figure 19.

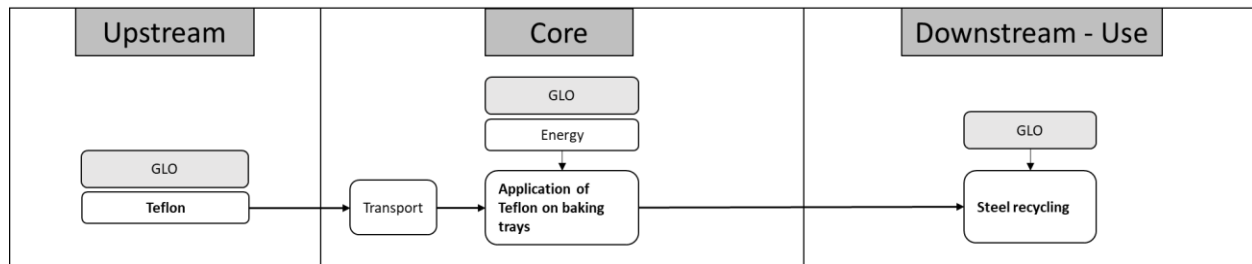


Figure 19 Upstream, Core and Downstream-Use of Teflon® baking tray according to LCA.

For the LCC and S-LCA of the benchmark, data was retrieved from the literature. As for the MCNM product, the benchmark life cycle stages included raw material sourcing, transportation, production energy, tray production, and usage (Figure 20). However, due to less specific literature data compared to industry information, the benchmark supply chain was simplified. Data primarily comes from the Ecoinvent database, with raw materials aggregated under a generic “Teflon®” process. The production stage is a single-phase including energy requirements. The benchmark product system aligns with the same three scenarios as the MCNM product system (Devecchi et al., In press). Indeed, both the main materials to produce the coating and the baking tray have three origin countries: China, USA and Europe. Cost sources are detailed in (Devecchi et al., In press). Figure 20 outlines the life cycle stages within the benchmark system boundaries. Due to limited information on the use stage for the benchmark, it is assumed that Teflon® application energy is the same as for the MCNM coating.

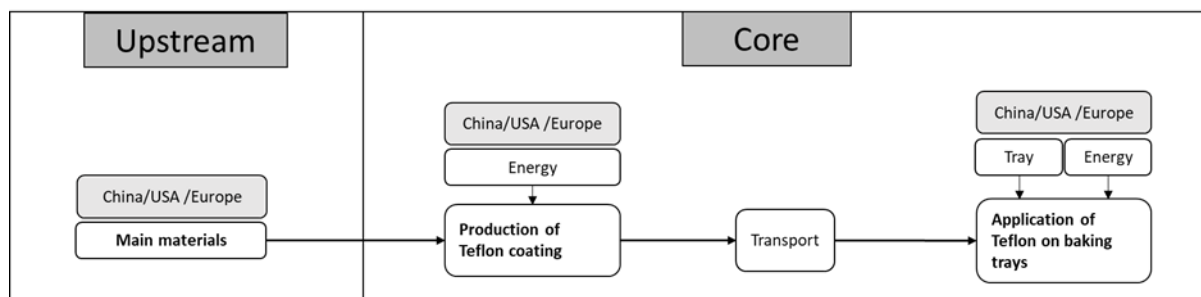


Figure 20 Upstream, Core and Downstream-Use of Teflon® baking tray according to LCC and S-LCA.

3.2.1.3. Life cycle inventory

For the LCA, LCC and S-LCA of the baking tray covered with anti-sticking coating, primary data were collected in 2023 through questionnaires filled in by the company that produces it. However, since the final anti-sticking coating is still in a design phase, some assumptions have been made. Indeed, full data will be available when the anti-sticking coating will be at a higher Technology Readiness Level (TRL).

In the next paragraphs, LCA, LCC and S-LCA related assumptions along with the processes selected from the databases both for the anti-sticking coating and the benchmark are reported.

LCA inventory

Anti-sticking coating

For the LCA study the assumptions made are the following:

- The means of transport on trucks used for the transportation of raw materials, main materials/components and the final product is: “Transport, freight, lorry 16-32 metric ton, EURO5 {RER}| transport, freight, lorry 16-32 metric ton, EURO5 | Cut-off, S”. from Ecoinvent 3.9.1.
- Ship transport for the transportation of raw materials such as Silica Carbide (SiC) 60nm, SiC 500nm, and of the anti-sticking coated baking trays for the maintenance is: “Transport, freight, sea, container ship {GLO}| transport, freight, sea, container ship | Cut-off, S” from Ecoinvent 3.9.1.

Table 8 reports all the LCA processes selected from the Ecoinvent database v3.9.1 to model raw materials, energy, transport sources and waste for the anti-sticking coated baking tray.

Table 8 LCA processes from Ecoinvent 3.9.1 database to model the anti-sticking coated baking tray.

Type	Raw materials	Process name in Ecoinvent 3.9.1 (Cut-off) database
Material	SiC 60 nm	Silicon carbide {RER} production

Material	SiC 500 nm	Silicon carbide {RER} production
Material	TiO2 shell precursor	Titanium dioxide {RER} production, sulfate/chloride process
Material	Isopropyl alcohol	Isopropyl acetate {RER} production
Material	Xylene solvent	Xylene {RER} production
Material	Silicone	Silicone product {RER} production
Material	Filler	Feldspar {RoW} production
Material	Water	Water, completely softened {RER} water production, completely softened
Material	Baking tray	Tin plated chromium steel sheet, 2 mm {GLO} market for
Energy	Electricity for production	Electricity, high voltage {ES} production mix
Energy	Electricity for the use	Electricity, high voltage {ES} production mix
Transport	Transport SiC 500 nm	Transport, freight, sea, container ship {GLO} transport, freight, sea, container ship Cut-off, S Transport, freight, lorry 16-32 metric ton, EURO5 {RER} transport, freight, lorry 16-32 metric ton, EURO5
Transport	Transport TiO2 shell precursor	Transport, freight, lorry 16-32 metric ton, EURO5 {RER} transport, freight, lorry 16-32 metric ton, EURO5
Transport	Transport Isopropyl alcohol	Transport, freight, lorry 16-32 metric ton, EURO5 {RER} transport, freight, lorry 16-32 metric ton, EURO5
Transport	Transport Xylene solvent	Transport, freight, lorry 16-32 metric ton, EURO5 {RER} transport, freight, lorry 16-32 metric ton, EURO5
Transport	Transport Silicone	Transport, freight, lorry 16-32 metric ton, EURO5 {RER} transport, freight, lorry 16-32 metric ton, EURO5
Waste	Cleaning water	Wastewater, average {RoW} treatment of, capacity 1E9l/year

Waste	Isopropyl alcohol	Spent solvent mixture {RoW} market for spent solvent mixture
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Benchmark

For the LCA study, the Ecoinvent database was used as source of data related to the baking tray coated with Teflon®. *Table 9* reports all the LCA processes selected from the Ecoinvent database v3.9.1 to model raw materials, energy, transports sources and waste for the baking tray covered with Teflon®.

Table 9 LCA processes from Ecoinvent 3.9.1 database to model the Teflon® coated baking tray.

Type	Raw materials	Process name in Ecoinvent 3.9.1 (Cut-off) database
Material	Teflon®	Tetrafluoroethylene {GLO} market for
Material	Baking tray	Tin plated chromium steel sheet, 2 mm {GLO} market for
Energy	Electricity for production	Electricity, high voltage {GLO} market group for electricity, high voltage
Energy	Electricity for the use	Electricity, high voltage {GLO} market group for electricity, high voltage
Waste	End i-of-life	Steel and iron (waste treatment) {GLO} recycling of steel and iron

LCC inventory

Anti-sticking coating

Unlike LCA and S-LCA, in LCC no processes are selected from a database but the costs related to the final product are used. Indeed, producing the baking tray coated with the anti-sticking coating involves several costs. These include the cost of the main materials and components, along with their transportation costs. Additionally, there are the costs of energy, waste collection and treatment, water used, and the maintenance of equipment, which are covered by the producer.

Since costs cannot be disclosed, the results will be presented as a percentage comparison of the costs of the MCNM coated baking tray against the benchmark.

Benchmark

As previously stated, due to insufficient data on the costs associated with the benchmark processes, which underpin both LCC and S-LCA analyses, three scenarios have been modeled:

- scenario 1 representing a benchmark produced in Europe;
- scenario 2 representing a benchmark produced in China;
- scenario 3 representing a benchmark produced in the USA.

The development of different production scenarios was unnecessary in the LCA presented above, as the Ecoinvent database, which was used to model the benchmark, already includes a “Tetrafluoroethylene GLO” process. This process accounts for the average global impacts associated with the material's production. The costs of the benchmark are reported in Annex 4.

S-LCA inventory

Anti-sticking coating

The social impacts along the supply chain of the assessed materials are modeled using the Social Hotspot Database (SHDB) available for SimaPro. This requires data on costs and the country of origin of main materials, transport, energy, and water consumption. Inputs in US Dollars 2011 were converted to euros using a factor of 1.392 to account for inflation when necessary (Devecchi et al., In press). Site-specific quantitative primary data were collected, covering the main material types, their amounts and costs, the resources required, and their countries of origin.

Table 10 reports all the S-LCA processes selected from the SHDB to model raw materials, water and energy sources for the baking tray covered with the anti-sticking coating.

Table 10 S-LCA processes from SHDB database to model the anti-sticking coated baked tray.

Type	Raw materials	Process name in SHDB

Material	SiC 60 nm	Mineral products nec/CHN S
Material	SiC 500 nm	Mineral products nec/CHN S
Material	TiO2 shell precursor	Metal products/GBR S
Material	Baking tray	Metal products/GBR S
Material	Isopropyl alcohol	Chemical, rubber, plastic products/ESP S
Material	Xylene solvent	Chemical, rubber, plastic products/ESP S
Material	Silicone	Mineral products nec/DEU S
Material	Filler	Mineral products nec/ESP S
Energy	Electricity for production	Electricity/ESP S
Energy	Electricity for use	Electricity/ESP S
Transport	Transport SiC 60 nm	Transport nec/CHN S
Transport	Transport SiC 500 nm	Transport nec/CHN S
Transport	Transport TiO2 shell precursor	Transport nec/GBR S
Transport	Transport Isopropyl alcohol	Transport nec/ESP S
Transport	Transport Xylene solvent	Transport nec/ESP S
Transport	Transport Silicone	Transport nec/DEU S
Transport	Transport Filler	Transport nec/ESP S

Benchmark

For the benchmark, the company that produces the anti-sticking coating conducted a review of Teflon® production countries and costs, integrated with the authors' research. The Ecoinvent database was the primary source of quantitative data on mass and energy requirements for Teflon® production, collected from Tetrafluoroethylene processes. For the Europe-based scenario, it was possible to identify the countries involved in sourcing and production from the

database unit process, aligning the selected European countries in the SHDB with the Ecoinvent inputs. Conversely, the global Tetrafluoroethylene process was too complex for geographical data extraction to be used for the China and USA-based scenarios. A literature review indicated that the main production actors are now located in the Pacific Asia region (Markets and Markets report, 2023). Therefore, SHDB processes from China were used for the first scenario, and from the USA for the second. This decision was because most major Teflon® industries originated in the USA, even though production has shifted to Asia in recent years (OECD, 2015). Despite this shift, the USA scenario remains relevant, providing an opportunity to highlight potential recent changes in social impacts due to relocation.

Table 11 reports all the S-LCA processes selected from the SHDB to model raw materials, water and energy sources for the baking tray covered with Teflon®. To avoid being redundant, the same processes were not reported 3 times in the table, each time with reference to a different country, rather they were reported only once and the different geographical location chosen for the processes were reported in the “Country” column.

Table 11 S-LCA processes from SHDB database to model the Teflon® baked tray.

Type	Raw materials	Process name in SHDB	Country
Material	PTFE	Chemical, rubber, plastic products	CHN / USA / RER
Material	Baking tray	Metal products	CHN / USA / RER
Energy	Natural gas	Gas	CHN / USA / RER
Energy	Electricity for use	Electricity	CHN / USA / RER
Transport	Transport	Transport nec	CHN / USA / RER

3.2.1.4. Life Cycle Impact Assessment

LCA, LCC and S-LCA were carried out with the use of the SimaPro LCA software developed by PRé Sustainability. ReCiPe 2016 Endpoint and Midpoint methods were used to calculate environmental impacts, while Categories and Subcategories methods were used to calculate social impacts. As the methods do not include characterization factors specific for nanoparticles

release (Salieri et al. 2019), for the LCA and S-LCA nanomaterials were modelled as bulk materials. In the next paragraphs, LCA, LCC and S-LCA results are reported.

LCA

The following section presents a comparative LCA of 1 m² of an industrial baking tray coated with the anti-sticking coating and 1 m² of an industrial baking tray coated with Teflon®, both evaluated over a five-year usage period. The results are presented at both the Midpoint and Endpoint levels. Midpoint results are shown in Table 12 as characterized results while Figure 21 illustrates the same results as percentages, with each impact category set to 100%. For each impact category, the most relevant contribution is clearly provided by the Teflon® coated tray.

Table 12 Midpoint characterization results of the anti-sticking coated baked tray and the Teflon®-coated tray.

Impact category	Anti-sticking coating baked tray	Teflon® coated tray	Unit
Global warming	150.3191	516.6518	kg CO2 eq
Stratospheric ozone depletion	7.36E-05	0.001447	kg CFC11 eq
Ionizing radiation	8.713533	29.87494	kBq Co-60 eq
Ozone formation, Human health	0.41699	1.196792	kg NOx eq
Fine particulate matter formation	0.391524	1.645623	kg PM2.5 eq
Ozone formation, Terrestrial ecosystems	0.429194	1.234138	kg NOx eq
Terrestrial acidification	0.516909	1.85774	kg SO2 eq
Freshwater eutrophication	0.064315	0.264393	kg P eq
Marine eutrophication	0.003038	0.013091	kg N eq
Terrestrial ecotoxicity	3570.387	13270.3	kg 1,4-DCB
Freshwater ecotoxicity	9.407577	41.80357	kg 1,4-DCB
Marine ecotoxicity	13.92212	60.19621	kg 1,4-DCB

Human carcinogenic toxicity	146.4949	721.6814	kg 1,4-DCB
Human non-carcinogenic toxicity	185.2885	744.2955	kg 1,4-DCB
Land use	6.080673	16.33594	m2a crop eq
Mineral resource scarcity	8.183403	40.35079	kg Cu eq
Fossil resource scarcity	42.16428	114.4779	kg oil eq
Water consumption	1.21456	5.212561	m3

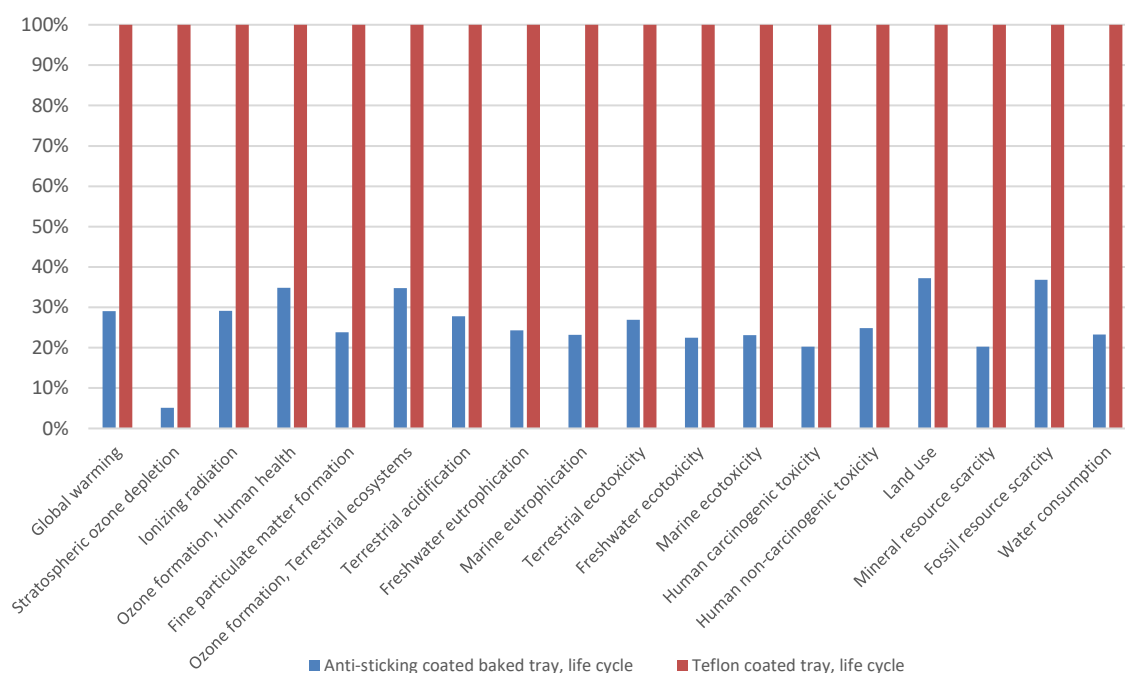


Figure 21 Midpoint characterization results of the anti-sticking coated baked tray and the Teflon®-coated tray.

To better understand the main contributors to the final impact, a detailed assessment was conducted. For both the baking trays coated with the anti-sticking coating and the Teflon®, various contributions such as energy required, materials and their transport, the baking tray itself, and waste treatment have been evaluated (Figure 22). Since the amount of material used to produce the baking tray is significantly greater than that used for the anti-sticking coating and the Teflon®, it was considered as a separate category to ensure visibility of the material impacts. Additionally,

the impacts related to the materials and their transport for the anti-sticking coating were grouped, as Teflon® lacks this differentiation, making the results otherwise incomparable.

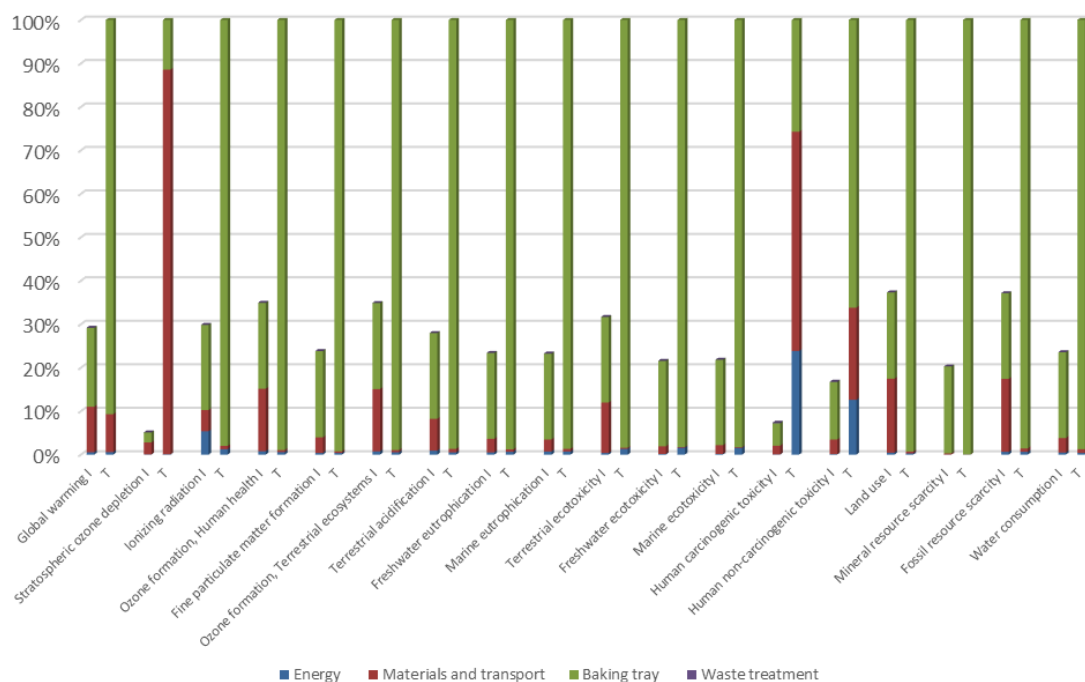


Figure 22 Midpoint characterization results of the anti-sticking coated baked tray (I) and the Teflon®-coated baking tray (T), with contributions showed for energy, materials and transports, baking tray and the waste treatment. To avoid redundancy, the full names of the impact categories are provided only for the innovative material, while a “T” is used for the same impact categories related to Teflon®.

From Figure 22 it is possible to see that the highest contribution for both the alternatives is given by the baking tray for all the impact categories, except for Stratospheric ozone depletion and Human carcinogenic toxicity impact categories. Indeed, for these two categories the highest contribution is given by the materials and their transport. Also, it is worth noting that the impact of the baking tray in the alternative using the innovative material, the anti-sticking coating, is lower compared to the one using the benchmark for all the impact categories. Endpoint results provide an overview of damages to *human health*, *ecosystems* and *resources*, caused by the life cycle of both the baking tray coated with the anti-sticking coating and the baking tray coated with Teflon®. The normalized results of the three endpoint indicators are reported in Figure 23. Similar to the midpoint results, the largest contributions to the calculated damages are related to the

benchmark. Furthermore, the most relevant endpoint is the damage to *human health* both for the anti-sticking coated and the Teflon® coated baked tray.

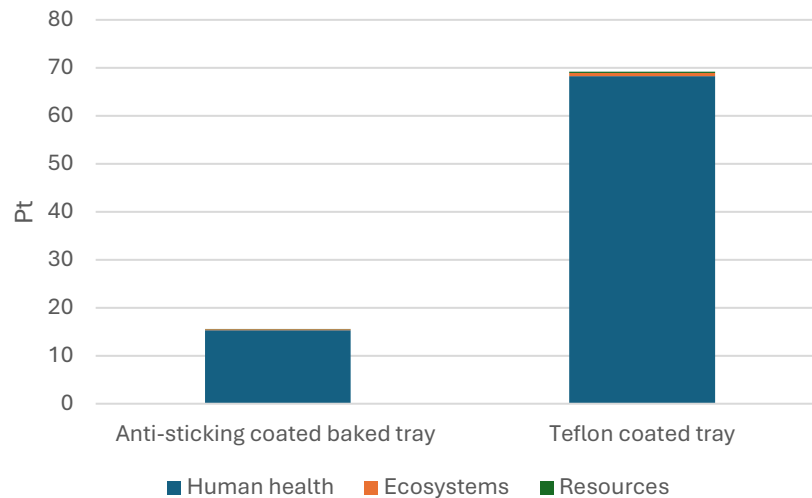


Figure 23 Endpoint results of the comparison between the anti-sticking coated baked tray and the Teflon®-coated tray.

LCC

In this paragraph the LCC results for the anti-sticking coated baking tray compared to the Teflon® coated tray are presented. As previously mentioned, due to the absence of primary data on process costs for the benchmark, the latter was modelled according to three scenarios:

- scenario 1 representing a benchmark produced in Europe;
- scenario 2 representing a benchmark produced in China;
- scenario 3 representing a benchmark produced in the USA.

Figure 24 illustrates the aggregated LCC results for the anti-sticking coated baking tray and the three benchmark scenarios, showing that the anti-sticking coating is the most cost-effective alternative, as the total life cycle costs of the baking tray coated with the innovative material are lower compared to those of the three benchmark's scenarios. Additionally, it is evident that among the three benchmark scenarios, the USA-based scenario has the highest impact, followed by the Chinese scenario, and lastly, the European scenario.

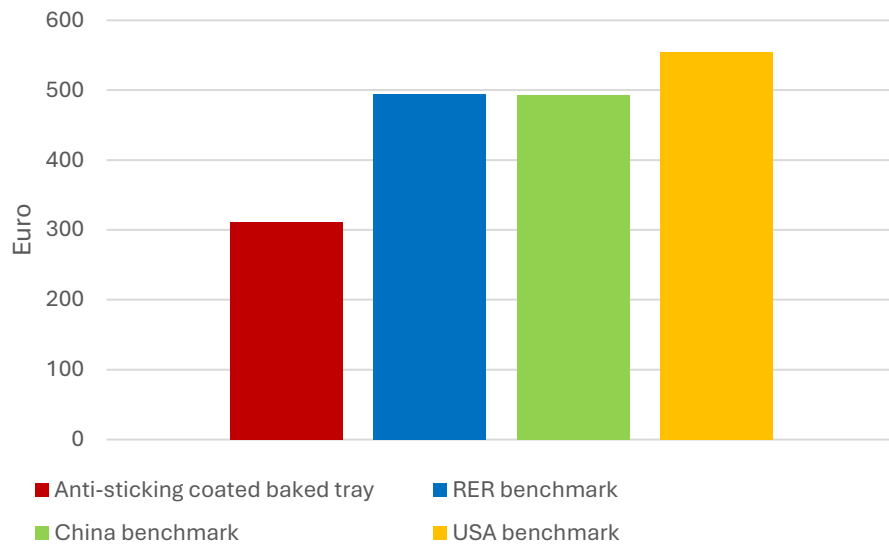


Figure 24 Aggregated costs result for the anti-sticking coated baked tray and the three benchmark's scenarios, China, Usa and Europe (RER)

Figure 25 presents the LCC results broken down by each cost category and scenario. In the three benchmark scenarios, the most significant cost category is the cost of the tray. This is followed by the cost of the main materials (i.e., the other materials used along the product lifecycle) in the USA scenario, whereas in the China and Europe scenarios, the next major cost is the end-of-life treatment. For the anti-sticking coated baking tray alternative, the highest cost is associated with transport to the maintenance facility, which surpasses all other costs. This is followed by the cost of the tray.

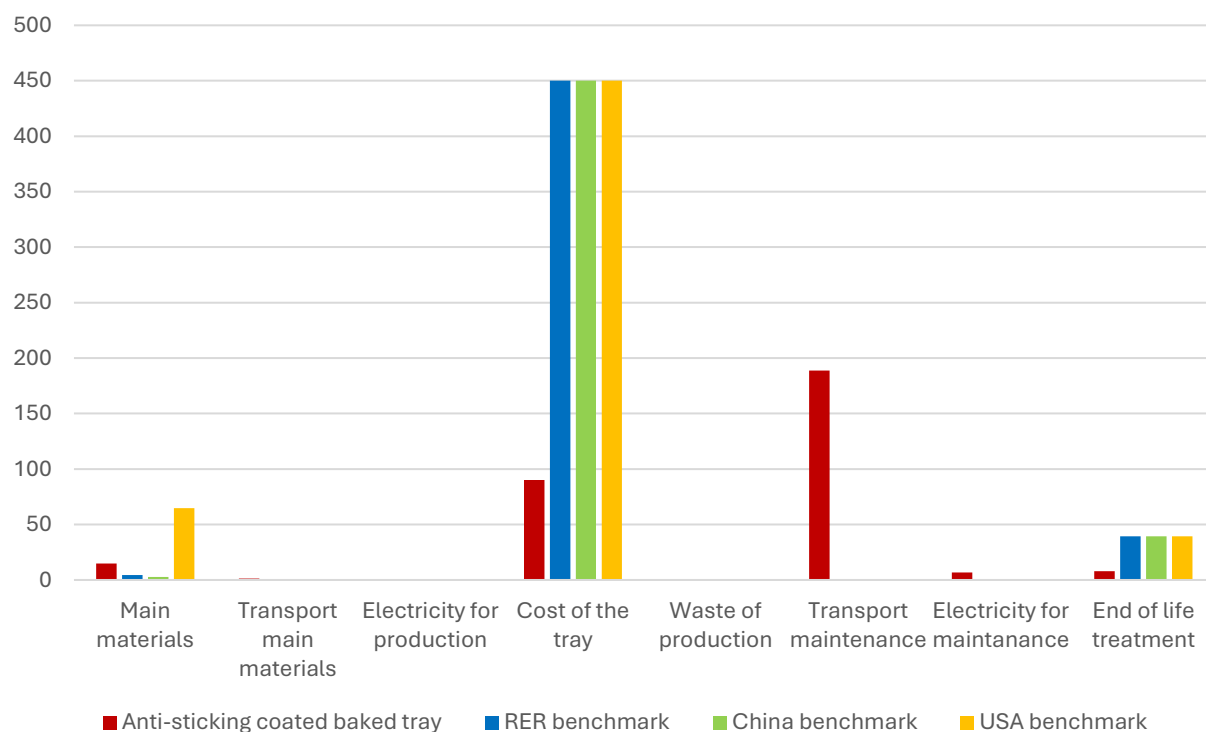


Figure 25 Disaggregated LCC results for the anti-sticking coated baked tray and the three benchmark scenarios

S-LCA

In this section, the potential social impacts of the anti-sticking coated baking tray are compared to those of the three benchmark scenarios. Figure 26 presents at the level of subcategories the results of the comparison between the innovative anti-sticking coating and the benchmark, according to the three scenarios and the 5 years life cycle considered in all the assessments. These results are obtained using the Social Hotspot 2016 Subcategory Method w Weights available in SHDB for SimaPro. The social impacts are represented on a scale of medium risk hours equivalent (mrheq). The baking tray coated with the innovative material performs better in all scenarios. The subcategories associated with the highest mrheq are Freedom of association and Occupational toxicity and hazard. Table 13 lists the impact subcategories associated with the codes in Figure 26.

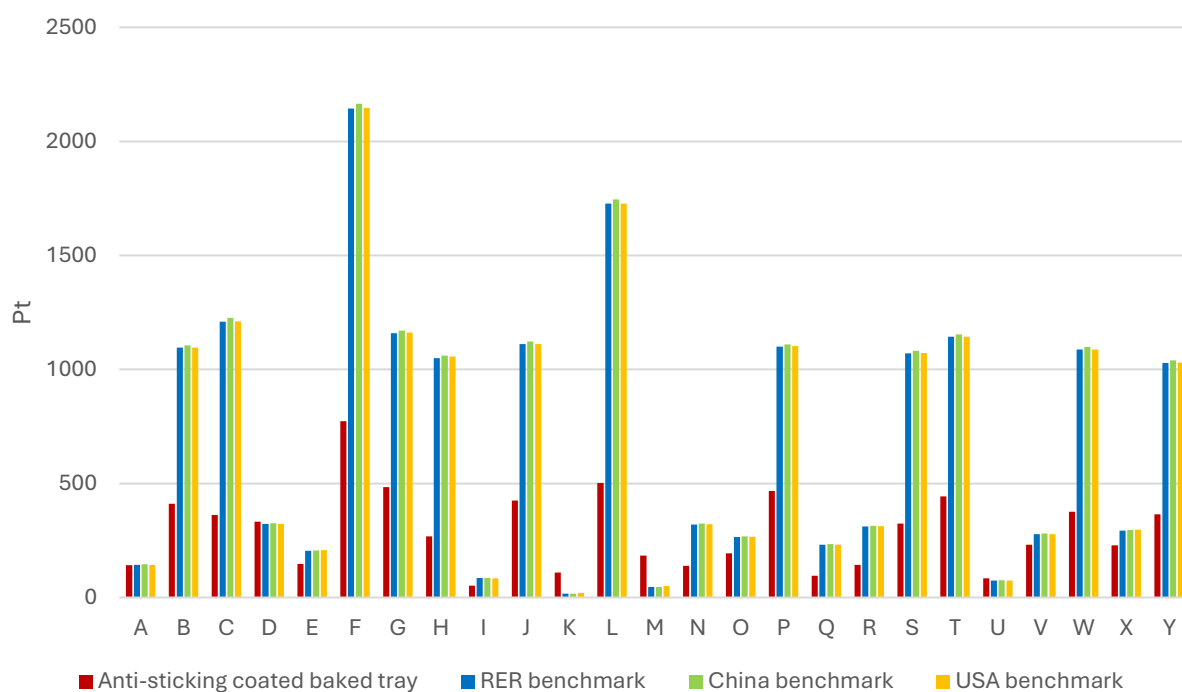


Figure 26 Social impact subcategories characterization results for the anti-sticking coated baked tray and the benchmark (Teflon® coated baking tray) scenarios. Pt= points. The unit is used to weight the result, augmenting or lowering the number of workers hours depending of the risk level probability.

Table 13 impact subcategories associated with the codes in Figure 26.

Impact category	code
Wage	A
Poverty	B
Child Labor	C
Forced Labor	D
Excessive Working Time	E
Freedom of Associaton	F
Migrant Labor	G
Social Benefits	H
Labor Laws/Conventions	I
Discrimination	J
Unemployment	K
Occupational Toxicity & Hazard	L
Injuries & Fatalities	M
Indigenous Rights	N
Gender Equity	O
High Conflict Zones	P
Non-Communicable Diseases	Q
Communicable Diseases	R
Legal System	S
Corruption	T
Access to Drinking Water	U
Access to Sanitation	V

Children out of School	W
Access to Hospital Beds	X

Figure 26 demonstrates that out of twenty-five subcategories, the anti-sticking coated baking tray has a lower social impact compared to the three benchmark scenarios in twenty-one categories. Specifically, the China benchmark scenario exhibits the highest impact in nineteen subcategories, while the USA benchmark scenario shows the highest impact in the remaining two subcategories, i.e. Excessive working time and Access to hospital beds, labelled “E” and “X” respectively. Among the three benchmarks, the European scenario consistently has a lower impact and never registers the highest impact in any category. In contrast, for the four remaining subcategories, Forced Labor, Unemployment, Injuries & Fatalities and Access to Drinking Water labelled "D," "K," "M," and "U" respectively, the anti-sticking coated baking tray shows a higher impact than the benchmark scenarios. In Figure 27 are the results of the aggregation of the subcategories into broader issues or at the categories level. Results by categories are obtained using the Social Hotspot 2016 Category Method w Weights available in SHDB for SimaPro. Since it can be compared to the endpoint level of the ReCiPe method for environmental LCA, results are less robust as conversion to impact categories involves approximation. The most affected categories are Health and Safety and Governance. The alternatives’ results are in line with those at subcategories level, showing lower impacts for the baking tray coated with the innovative product in all the categories, and similar results for the three benchmark scenarios.

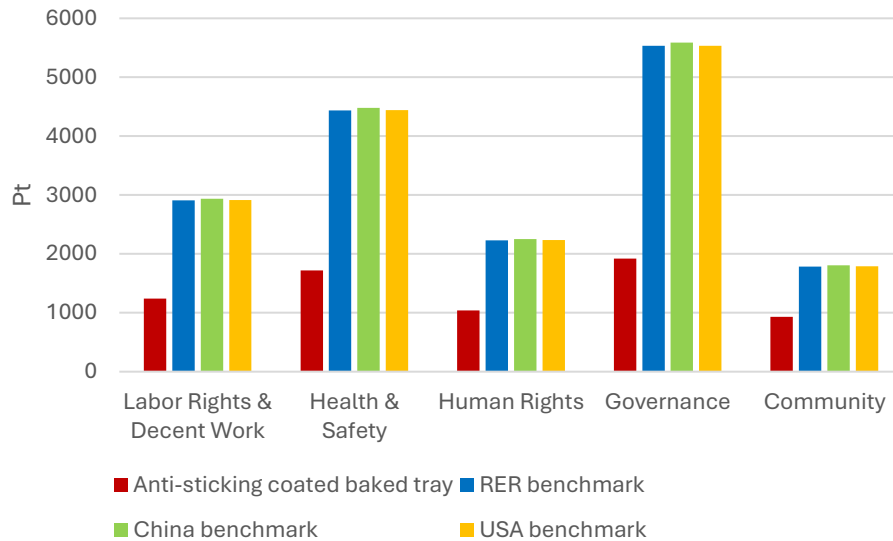


Figure 27 Categories weighting results for the anti-sticking coated baked tray and the benchmark (Teflon®) coated baking tray according to the three scenarios. Pt= points. The unit is used to weigh the result, augmenting or lowering the number of workers hours depending on the risk level probability

3.2.2.Active food packaging

3.2.2.1. Goal and scope definition

The goal of LCA, LCC and S-LCA was to minimise the environmental impacts of the active food packaging, a MCNM-functionalized packaging, described in Chapter 1.3 while optimising its social and economic cost-benefit ratio.

The functional unit selected is 31.04 tonnes of cereals sold to the retailers, which after harvesting have been stored either in the MCNM-functionalized packaging or in traditional packaging. The amount was chosen based on the amount of kgs of functionalized packaging the company provided. Packaging can be either made of low-density polyethylene (LDPE) or biopolymer, resulting in four options: 1) MCNM-functionalized LDPE packaging, 2) LDPE packaging, 3) MCNM-functionalized biopolymer packaging, and 4) biopolymer packaging. LDPE packaging and biopolymer packaging have been considered benchmarks. In the storage period of the traditional packaging, it is assumed that there will be a loss of 20% of the cereals due to pests (Kumar & Kalita, 2017), while for the active food packaging option, the loss was assumed as 0%. The storage conditions are not considered, as well as the transportation from the harvesting to the storage facilities, due to lack of data.

3.2.2.2. System boundaries

In the following paragraphs, the system boundaries of the active food packaging and of the benchmark are described.

Active food packaging

Based on information obtained from the company that produces the active food packaging, the product system for this innovative packaging functionalized with nanodrops of essential oil anchored at the surface of nano-clays was modelled within the software SimaPro. The diagram of the system under assessment is illustrated in Figure 28.

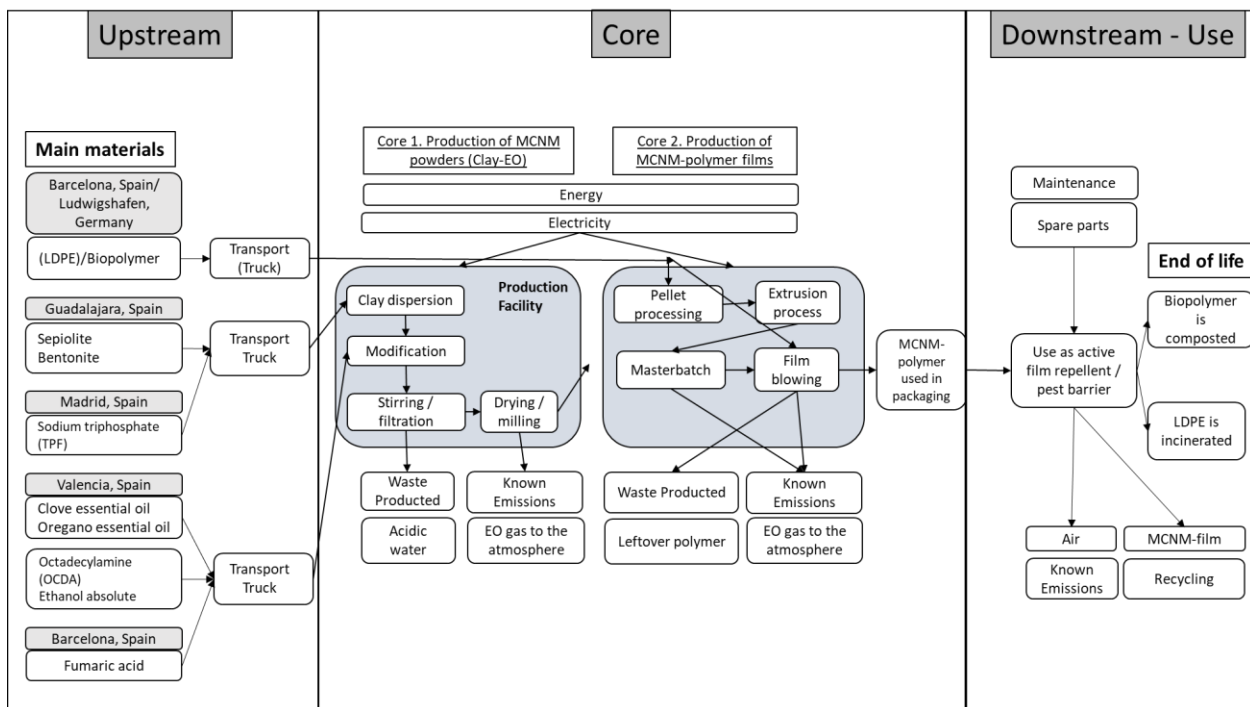


Figure 28 Upstream, Core and Downstream-Use of active food packaging.

In the LCA study, energy and matters flows related to the Upstream, Core and Downstream stages of an active food packaging functionalized with nanodrops of essential oil anchored at the surface of nano-clays are considered. As shown in Figure 28, the main materials were purchased mostly from Spain, except for a German supplier. From these countries, the main materials were transported by truck to Castellon (Spain) where the manufacturing core process of the

functionalized clay powder and the MCNM-polymer films takes place. The functionalized nano-clays are produced with materials such as bentonite, sepiolite, sodium triphosphate, clove and oregano essential oils, octadecylamine, ethanol absolute, and fumaric acid. Four versions of the nano-clay are produced, combining the two types of essential oils with either sepiolite or bentonite. Due to the limitation of the database used, in the assessment, it is considered only one version of the MCNM clay, produced with bentonite and a generic essential oil. The production facility, in the Core stage, involves eight main processes, four to produce the functionalized clay powder and four for the MCNM-polymer films. The polymer films can be either made of low-density polyethylene (LDPE) or a biopolymer. Respectively, the main processes are clay dispersion, modification, stirring/filtration, and drying/milling; pellet processing, extrusion process, masterbatch, and film blowing. As depicted in Figure 28, at Core stage, used electricity and produced waste are considered. At the end of the production, the MCNM-polymer film is shipped from Castellon to any country that needs it. Since the MCNM-polymer film is in the design stage, its end-of-life is assumed to be either an incineration process, if plastic, or composting, if biopolymer.

For the LCC and S-LCA, the costs relative to Upstream (i.e., main materials/components and their transport), Core (i.e., production of the functionalized clay powder and the MCNM-polymer films), and Downstream (i.e., use as a packaging for cereals) stages were considered. The end-of-life (i.e., incineration or recycling), part of the Downstream stage, was considered only for the LCC since the S-LCA database (SHDB) still has no waste disposal process available. The shipment costs to other countries were not available and, therefore, were not included in the assessment.

Benchmark

For the LCA, the benchmark considers the same raw material to produce the active food packaging, without those to produce the MCNM. Therefore, only the processes to produce traditional LDPE packaging and traditional biopolymer packaging are considered. For the LCA, the processes for both the benchmarks are included within the Ecoinvent database. In contrast, the S-LCA faced challenges due to the absence of active food packaging process in the Social Hotspots

Database (SHDB). Additionally, the LCA considers the end-of-life phase of the product, whereas the S-LCA does not, as the SHDB currently lacks waste disposal processes.

For the LCA of the benchmark, both the LDPE and biopolymer packaging, data from the Ecoinvent database served as the primary reference. This included the LDPE and biopolymer materials, the process required to extrude the granulate of LDPE and biopolymer and the waste treatment of LDPE. The diagram of the system under assessment according to the LCA is illustrated in Figure 29

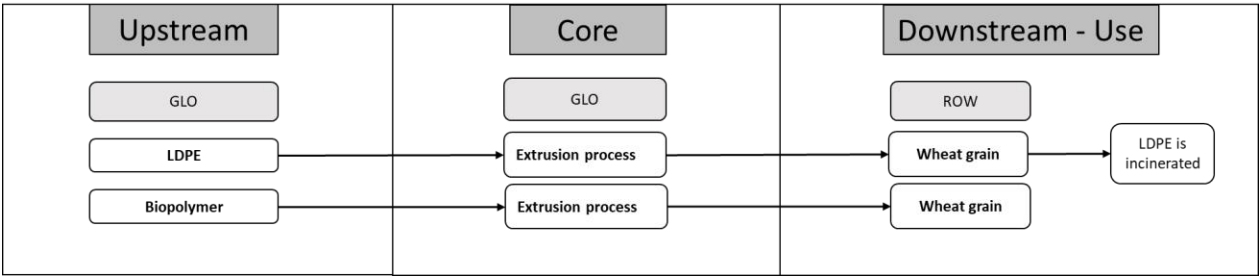


Figure 29 Upstream, Core and Downstream-Use of LDPE and biopolymer packaging according to LCA.

For the LCC and S-LCA of the benchmark, data was retrieved from the literature. Due to less specific literature data compared to industry information, the benchmark supply chain is simplified. Data primarily comes from the Ecoinvent database, with raw materials aggregated under a generic “LDPE” process. The benchmark product system aligns with the same scenario as the active food packaging product system. Figure 30 outlines the life cycle stages within the benchmark system boundaries.

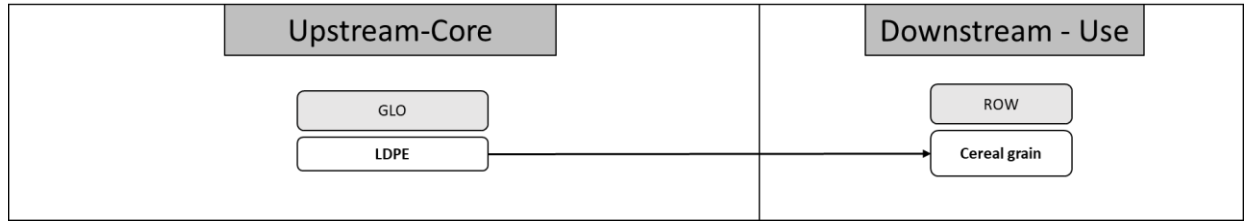


Figure 30 Upstream, Core and Downstream-Use of LDPE packaging according to LCC and S-LCA.

3.2.2.3. Life cycle inventory

For both LCA, LCC and S-LCA of the active food packaging, primary data were collected in 2023 through questionnaires filled in by the company that produces it. However, since the final MCNM

is still in a design phase, some assumptions have been made. Indeed, full data will be available when the MCNM is at higher Technology Readiness Level (TRL).

In the next paragraphs, LCA, LCC and S-LCA related assumptions along with the processes selected from the databases both for the active food packaging and benchmark, are reported.

LCA inventory

Active food packaging

For the LCA study the assumptions made are the following:

- The means of transport by truck used for the transport of raw materials, main materials/components and the final product is: “Transport freight, lorry >32 metric ton, EURO6 {RER}| transport, freight, lorry >32 metric ton” from Ecoinvent 3.9.1.
- The Bentonite was selected as a German process since the only available options were a German or a Rest of the World geographies. The choice is due to the assumption that a German option might have similar impacts of a Spanish one, due to the common policies of EU in terms of chemical production.
- The essential oil was modelled thanks to the HD scenario provided by (Moura et al., 2022). The plant process selected from the database is Mint {RoW}| mint production | Cut-off since it was the only option also known as an essential oil product.
- The Sodium triphosphate (TPF) was associated with a phosphoric acid database process since it was not available a more specific project. Indeed, TPF is the sodium salt of polyphosphate penta-anion, which is the conjugate base of triphosphoric acid. This is a condensed form of the phosphoric acid, chosen as a proxy for the model.
- The octadecylamine (OCDA) was associated with a steric acid database process since it is the product of hydrogenation of stearyl nitrile, derived from stearic acid and nitrile (OMRI, 2001).

- Fumaric acid was associated with a maleic anhydride database process. Indeed, Fumaric acid is currently produced by isomerization of maleic acid, which is produced from maleic anhydride (Roa Engel et al., 2008).
- The MCNM-polymer film and its components were considered in their entirety and used with their background in the evaluation of impacts (Table 14).
- The process of production of the LDPE and biopolymer packaging was modelled considering a process of injection moulding for both the innovative product and the benchmark.
- The recycling of the biopolymer packaging was modelled with a treatment of Polyethylene (PE) due to a lack of specific recycling processes. However, for the system model adopted, the cut-off by classification, the impacts of the recycling are not bore by the producer of the waste, but to the user. Therefore, the association with a non-specific process does not significantly change the results of the assessment.

Table 14 reports all the LCA processes selected from the Ecolnvent database v3.9.1 to model raw materials, energy, transport sources and waste.

Table 14 LCA processes from Ecolnvent 3.9.1 database to model the active food packaging.

Type	Raw materials	Process name in Ecolnvent 3.9.1 (Cut-off) database
Material	Bentonite	Activated bentonite {DE} activated bentonite production Cut-off, S
Material	Generic essential oil	Essential oil
Material	Sodium triphosphate (TPF)	Phosphoric acid, industrial grade, without water, in 85% solution state {RER} purification of wet-process phosphoric acid to industrial grade, product in 85% solution state Cut-off, S
Material	Octadecylamine (OCDA)	Stearic acid {GLO} stearic acid production Cut-off, S Nitrile-compound {RER} nitrile-compound production Cut-off, S

Material	Ethanol absolute	Ethanol, without water, in 95% solution state, from fermentation {RER} ethanol production from rye Cut-off, S
Material	Sodium carbonate	Soda ash, light {RER} soda production, solvay process Cut-off, S
Material	Fumaric acid	Maleic anhydride {RER} maleic anhydride production by catalytic oxidation of benzene Cut-off, S
Material	Low density polyethylene (LDPE)	Polyethylene, low density, granulate {RER} polyethylene production, low density, granulate Cut-off, S
Processing	Extrusion of LDPE and biopolymer	Extrusion, plastic film {GLO} market for extrusion, plastic film Cut-off, S
Material	Biopolymer	Polyester-complexed starch biopolymer {RER} polyester-complexed starch biopolymer production Cut-off, S
Material	Cereal	Wheat grain {RoW} market for wheat grain Cut-off, S
Water	Water	Water, completely softened {RER} market for water, completely softened Cut-off, S
Energy	Renewable	Electricity, medium voltage {ES} electricity voltage transformation from high to medium voltage Cut-off, S
Waste	Incineration of LDPE packaging	Waste polyethylene {RoW} treatment of waste polyethylene, municipal incineration Cut-off, S
Waste	Recycling of biopolymer packaging	PE (waste treatment) {GLO} recycling of PE Cut-off, S

Benchmark

For the LCA study the assumptions made are the following:

- When available, processes with a Global geography were used to avoid biases due to regionalization.

- The process of production of the LDPE and biopolymer packaging was modelled considering a process of injection moulding for both the innovative product and the benchmark.
- The recycling of the biopolymer packaging was model with a treatment of Polyethylene (PE) due to lack of specific recycling processes. However, for the system model adopted, the cut-off by classification, the impacts of the recycling are not bore by the producer of the waste, but to the user. Therefore, the association with a non-specific process does not significantly change the results of the assessment.

For the LCA study, the Ecoinvent database was used as a source of data related to the active food packaging. Table 15 reports all the LCA processes selected from the Ecoinvent database v3.9.1 to model raw materials, energy, transport sources and waste for the active food packaging.

Table 15 LCA processes from Ecoinvent 3.9.1 database to model the benchmark.

Type	Raw materials	Process name in Ecoinvent 3.9.1 (Cut-off) database
Material	Low-density polyethylene (LDPE)	Polyethylene, low density, granulate {GLO} polyethylene production, low density, granulate Cut-off, S
Material	Biopolymer	Polyester-complexed starch biopolymer {GLO} market for polyester-complexed starch biopolymer Cut-off, S
Material	Cereal	Wheat grain {RoW} market for wheat grain Cut-off, S
Processing	Extrusion of LDPE and biopolymer	Extrusion, plastic film {GLO} market for extrusion, plastic film Cut-off, S
Waste	Incineration of LDPE packaging	Waste polyethylene {RoW} treatment of waste polyethylene, municipal incineration Cut-off, S

LCC inventory

Active food packaging

The following costs of producing the active food packaging (i.e. upstream, core and downstream stage) were considered: i) cost of main materials and components, ii) the cost of their transportation, iii) cost of energy for the production, iv) cost of waste collection and treatment, v) cost of water used, vi) cost of cereal production. The costs of the extrusion process to produce the LDPE packaging or the biopolymer packaging were not included as they were not available. Due to the lack of primary data on the cost of cereals, which is necessary for both the LCC and the S-LCA, the average global cost was taken from the literature.

Benchmark

The benchmarks were modelled with the innovative products data since it was assumed that the price for the LDPE and the biopolymer packaging would coincide. Due to the lack of primary data on the cost of cereals, which is necessary for both the LCC and the S-LCA, the average global cost was taken from the literature.

S-LCA inventory

Active food packaging

The SHDB list of GTAP sectors does not include all the available ones. Manufacture of rubber and plastics products and Manufacture of chemicals and chemical products GTAP sectors are aggregated into one SHDB process “Chemical, rubber, plastic products”. Thus, it was decided to associate the LDPE to the “Petroleum, coal products” process, to differentiate from the MCNM manufacturing chemicals, pertaining to the aggregated category mentioned above. Indeed, the SHDB offers a limited number of processes, due to the relative recent interest the S-LCA methodology gained. For the same reason, it was decided to not include in the assessment the biopolymer options, since it does not exist a process that would allow to differentiate the results.

Table 16 shows the association of all the materials to SHDB processes. Indeed, since most materials are associated to the same type of process, the final results miss a level of detail that the SHDB cannot yet provide. Transport costs were included and aggregated into material costs provided by the MCNM production company. Therefore, they were allocated to processes based

on the assumption that transport usually accounts for 10% of the cost of the product (Rodrigue, 2024). Energy, even though renewable, could not be associated with a specific process, and therefore, it does not account for the benefits of utilizing renewable energy.

Table 16 Raw Materials and associated SHDB processes to model the active food packaging.

Type	Raw materials	Process name in SHDB
Material	Bentonite	Chemical, rubber, plastic products/ESP S
Material	Essential oil	Chemical, rubber, plastic products/ESP S
Material	Sodium triphosphate (TPF)	Chemical, rubber, plastic products/ESP S
Material	Octadecylamine (OCDA)	Chemical, rubber, plastic products/ESP S
Material	Ethanol absolute	Chemical, rubber, plastic products/ESP S
Material	Sodium carbonate	Chemical, rubber, plastic products/ESP S
Material	Fumaric acid	Chemical, rubber, plastic products/ESP S
Material	LDPE	Petroleum, coal products/ESP S
Material	Cereals	Cereal grains nec/ESP S
Transport	Truck	Transport nec/ESP S
Energy	Electricity, renewable	Electricity/ESP S
Water	Water	Water/ESP S

Benchmark

For the benchmark, the Ecoinvent database was the primary source of quantitative data on mass and energy requirements for LDPE and the biopolymer packaging production. As for the active food packaging, the LDPE process was associated with the “Petroleum, coal products” process. As previously mentioned, the SHDB offers a limited number of processes due to the relative recent interest the S-LCA methodology gained. As for the active food packaging, also for the

benchmark, it was decided not to include in the assessment the biopolymer options, since no process would allow to differentiate the results.

Table 17 reports all the S-LCA processes selected from the SHDB to model raw materials, water and energy sources.

Table 17 S-LCA processes from SHDB database to model the LDPE benchmark.

Type	Raw materials	Process name in SHDB
Material	Cereals	Cereal grains nec/ESP S
Material	LDPE	Petroleum, coal products/ESP S

3.2.2.4. Life Cycle Impact Assessment

LCA, LCC and S-LCA were carried out with the use of the SimaPro LCA software developed by PRé Sustainability. ReCiPe 2016 Endpoint and Midpoint methods were used to calculate environmental impacts, while Categories and Subcategories methods were used to calculate social impacts. As the methods do not include characterization factors specific for nanoparticle release (Salieri et al., 2018), nanomaterials were modelled as bulk materials for the LCA and S-LCA.

LCA

The following section presents a comparative LCA of the active food packaging, a MCNM-functionalized packaging, compared to a traditional benchmark food packaging. The results are presented at both the Midpoint and Endpoint levels. Midpoint results are shown in Table 18 as characterized results for each impact category for the four product lifecycles considered: the MCNM-functionalized LDPE, the LDPE benchmark, the MCNM-functionalized biopolymer, and the biopolymer benchmark.

In Figure 31, the same results are reported as percentages, where each impact category result is set at 100% and relative contributions of different product lifecycles are presented in different colours. The two benchmark product lifecycles are the most impactful due to the higher impact associated with cereal production. Indeed, to obtain the same quantity for the market, in these

cases a 20% more is required due to loss. Only for the ionizing radiation impact categories the Encapsulæ options provide the highest contribution.

Table 18 Midpoint characterization results of the comparison between the MCNM-functionalized LDPE, the LDPE benchmark, the MCNM-functionalized biopolymer, and the biopolymer benchmark packaging.

Impact category	MCNM-functionalized LDPE	LDPE benchmark	MCNM-functionalized biopolymer	Biopolymer benchmark	Unit
Global warming	25428.66642	28173.00131	25274.55286	27972.34639	kg CO ₂ eq
Stratospheric ozone depletion	0.340581809	0.403676336	0.340726193	0.403839802	kg CFC11 eq
Ionizing radiation	1587.747837	387.7316076	1584.936552	387.6166415	kBq Co-60 eq
Ozone formation, Human health	84.90173237	95.70325601	84.92104193	95.68931313	kg NO _x eq
Fine particulate matter formation	52.27929043	59.16463552	52.33094096	59.21970807	kg PM _{2.5} eq
Ozone formation, Terrestrial ecosystems	87.19879714	98.20446858	87.21358056	98.18183717	kg NO _x eq
Terrestrial acidification	260.307646	300.0284002	260.4651791	300.2163933	kg SO ₂ eq
Freshwater eutrophication	16.39875482	19.16675795	16.41067376	19.17262569	kg P eq
Marine eutrophication	63.30303916	74.59999126	63.32210919	74.62207649	kg N eq
Terrestrial ecotoxicity	79524.05677	91349.64958	79481.01935	91098.60033	kg 1,4-DCB
Freshwater ecotoxicity	886.9293961	1009.752004	878.9255838	999.7073816	kg 1,4-DCB
Marine ecotoxicity	1116.462901	1267.896506	1104.596919	1252.936779	kg 1,4-DCB
Human carcinogenic toxicity	997.5823816	1097.656764	999.5780363	1098.775108	kg 1,4-DCB

Human non-carcinogenic toxicity	23797.73357	27833.78517	23765.22322	27777.13179	kg 1,4-DCB
Land use	89027.98395	105863.7665	89039.35441	105877.1606	m2a crop eq
Mineral resource scarcity	128.3027017	147.6412792	128.5125593	147.8409787	kg Cu eq
Fossil resource scarcity	4191.977716	4372.974309	4164.424646	4333.918413	kg oil eq
Water consumption	6669.259717	7794.513835	6670.207862	7796.928269	m3

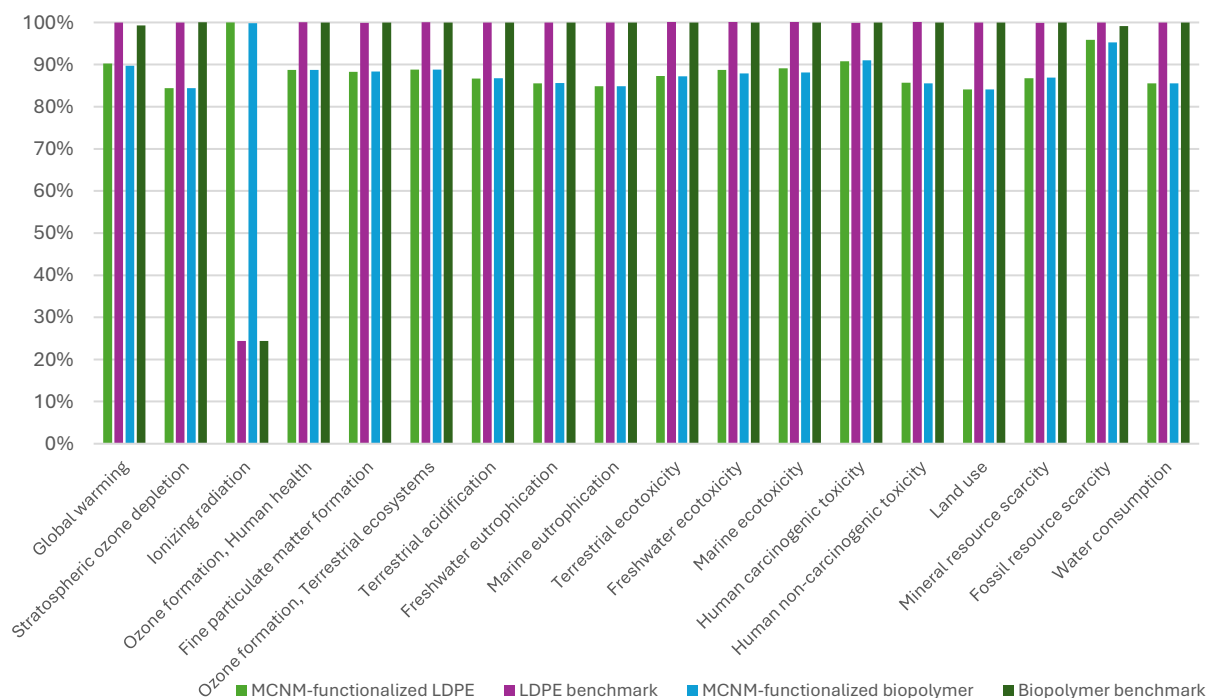


Figure 31 Midpoint characterization results of the comparison between the MCNM-functionalized LDPE, the LDPE benchmark, the MCNM-functionalized biopolymer, and the biopolymer benchmark.

Endpoint results provide an overview of damages to *human health*, *ecosystems* and *resources*, generated by the environmental impacts caused by the life cycle of the four product lifecycles considered: the MCNM-functionalized LDPE, the LDPE benchmark, the MCNM-functionalized biopolymer, and the biopolymer benchmark.

The normalized results of the three endpoint indicators are reported in Figure 32. Similar to the midpoint results, the largest contributions to the calculated damages are related to the benchmark products. The most relevant endpoint is *human health*, for the lifecycle of the four products.

The contribution of the life cycle of cereals is the most impactful on the damage category of *human health* and *Ecosystems*. Indeed, both the MCNM-functionalized LDPE and the MCNM-functionalized biopolymer options are associated with lower impacts. This depends to the reduced post-harvest food loss and therefore a lower input of cereals in their life cycles.

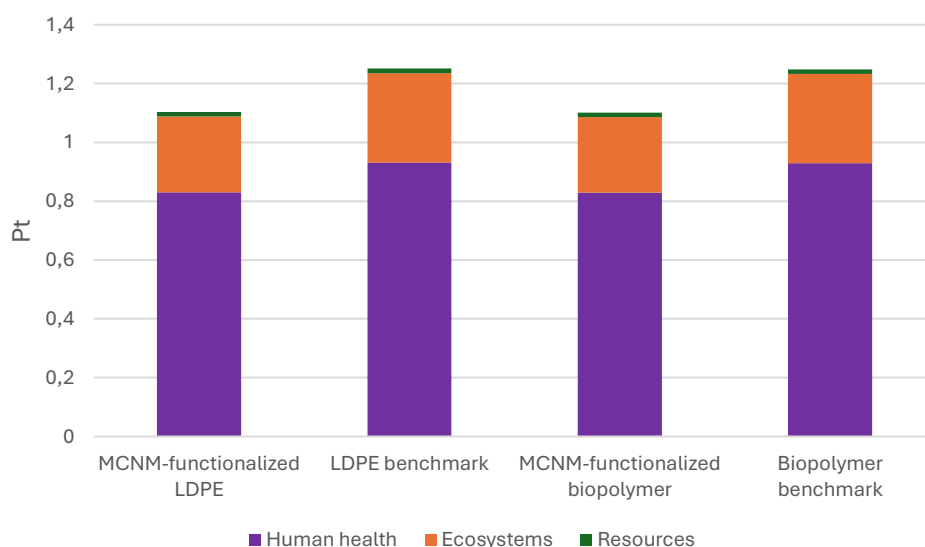


Figure 32 Endpoint results of the comparison between the MCNM-functionalized LDPE, the LDPE benchmark, the MCNM-functionalized biopolymer, and the biopolymer benchmark.

LCC

Figure 33 shows the LCC aggregated costs of the comparison between the MCNM-functionalized LDPE packaging, the LDPE benchmark, the MCNM-functionalized biopolymer, and the biopolymer benchmark. The cost of the benchmark's life cycle is higher than the MCNM-functionalized LDPE and the MCNM-functionalized biopolymer options. Figure 34 reports the prices disaggregated for each cost category and for each option. The most impactful category for the benchmark is the use phase, corresponding to the cereals production, due to the higher quantity lost for the benchmark option. In comparison to this phase, all the others have a very low impact.

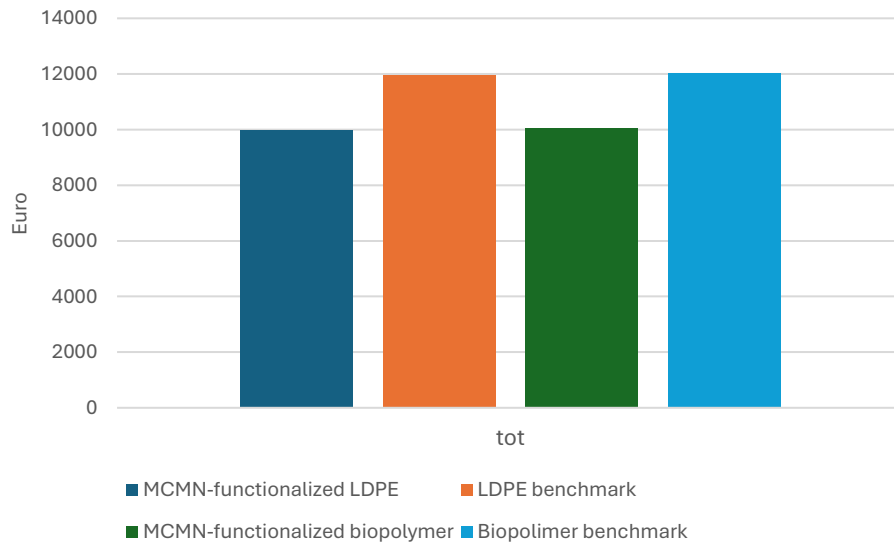


Figure 33 Aggregated costs results of the comparison of the life cycle of a LDPE/biopolymer MCNM-functionalized packaging with a traditional LDPE/biopolymer packaging.

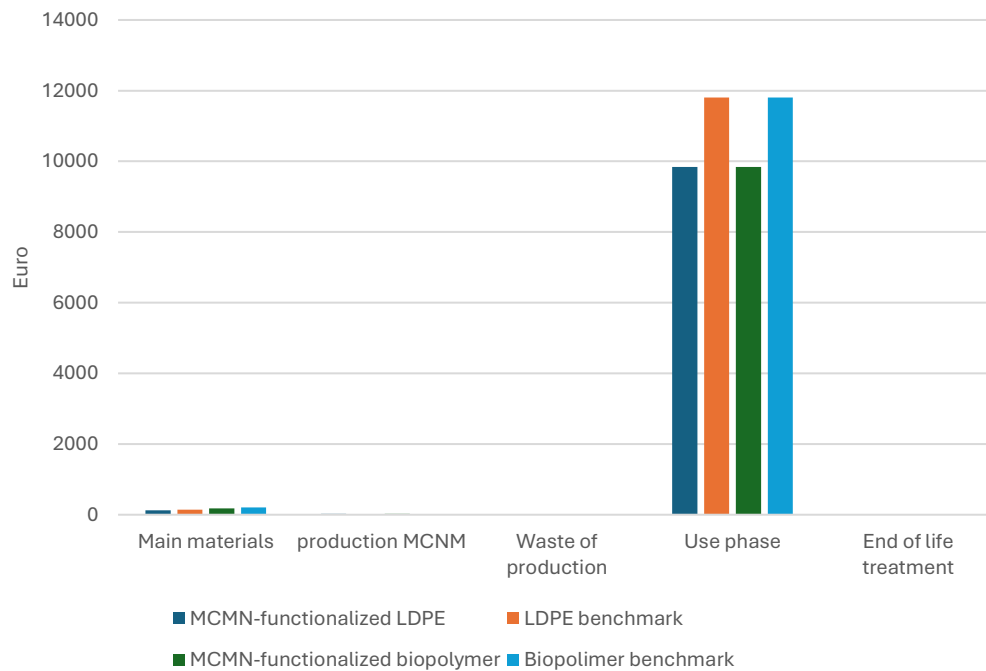


Figure 34 Disaggregated costs result of the comparison of the life cycle of a LDPE/biopolymer MCNM-functionalized packaging with a traditional LDPE/biopolymer packaging.

S-LCA

As mentioned in Chapter 2.3, both for the active food packaging and the benchmark, it was decided not to include the biopolymer options in the assessment since SHDB offers a limited number of processes. Therefore, results in Figure 35 show at the level of subcategories the comparison between the MCNM-functionalized and the benchmark. These results are obtained using the Social Hotspot 2016 Subcategory Method w Weights available in SHDB for SimaPro. The social impacts are represented on a scale of medium risk hours equivalent (mrheq). The MCNM-functionalized LDPE performs better due to the prevention of food loss and the social risks associated with the agricultural sector. The subcategories associated with the highest mrheq are freedom of association and Injuries & Fatalities. Table 19 lists the impact subcategories associated with the codes in Table 19.

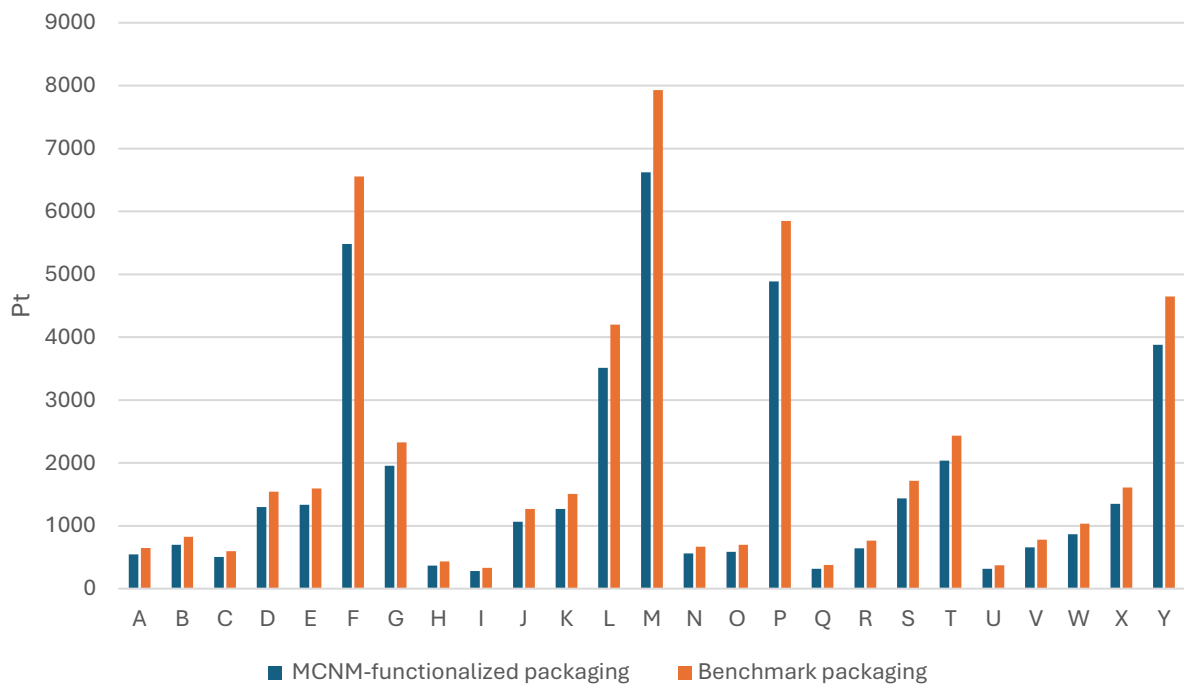


Figure 35 Social impact subcategories characterization results for the MCNM-functionalized packaging and the benchmark. Pt= points. The unit is used to weight the result, augmenting or lowering the number of workers hours depending on the risk level probability.

Table 19 impact subcategories associated with the codes in Figure 35.

Impact category	code
Wage	A
Poverty	B
Child Labor	C
Forced Labor	D
Excessive Working Time	E
Freedom of Association	F
Migrant Labor	G
Social Benefits	H
Labor Laws/Conventions	I
Discrimination	J
Unemployment	K
Occupational Toxicity & Hazard	L
Injuries & Fatalities	M
Indigenous Rights	N
Gender Equity	O
High Conflict Zones	P
Non-Communicable Diseases	Q
Communicable Diseases	R
Legal System	S
Corruption	T
Access to Drinking Water	U
Access to Sanitation	V
Children out of School	W
Access to Hospital Beds	X

Figure 36 shows the results of the aggregation of the subcategories at the categories level. Results by categories are obtained using the Social Hotspot 2016 Category Method w Weights available in SHDB for SimaPro. Since this method can be compared to the endpoint level of the ReCiPe method for environmental LCA, results are less robust as conversion to impact categories involves approximation. The category most affected is Health and Safety. The scenarios' results agree with

the results at the levels of subcategories, showing lower impacts for the MCNM-functionalized packaging in all the categories.

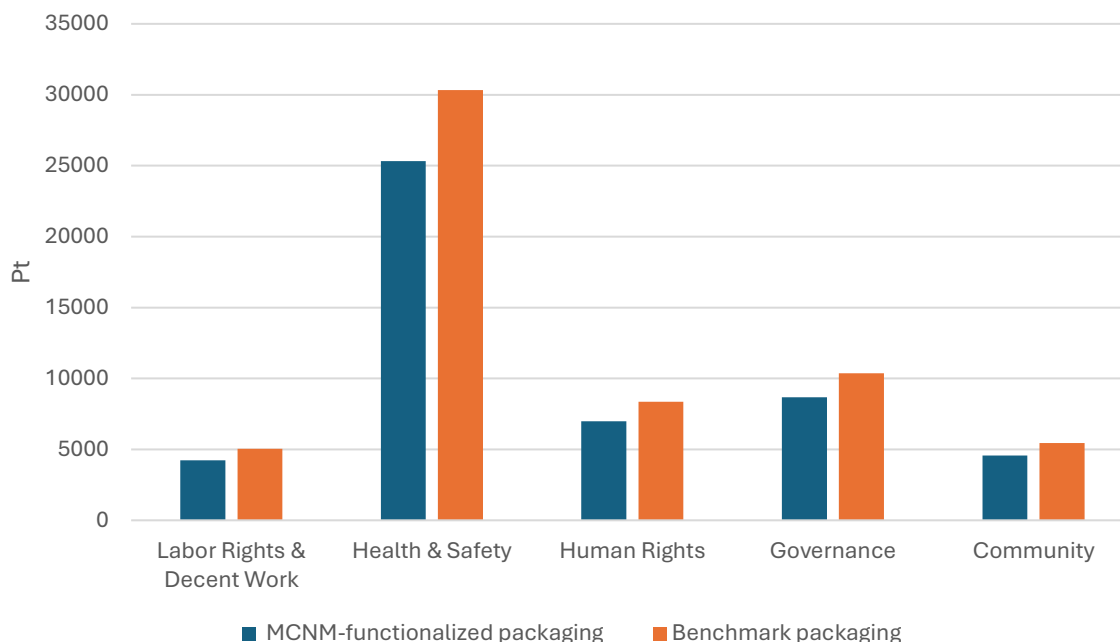


Figure 36 Category weighting results for the comparison between the MCNM-functionalized packaging and the benchmark. Pt= points. The unit is used to weight the result, augmenting or lowering the number of workers hours depending on the risk level probability.

3.2.3.ACRE TFT

3.2.3.1. Goal and scope definition

The goal of the cradle-to-gate LCA was to minimise the environmental impacts of an ACRE Thin-film-transistor (TFT). The selected functional unit (FU) was the production of 1 transistor. In the study, the impacts of the use of the transistor are not considered as well as the end of life, since a cradle-to-gate assessment is carried out. Data for the benchmark (nome del benchmark) comes from LCA database processes and literature review.

3.2.3.2. System boundaries

In the following paragraphs, the system boundaries of the ACRE TFT and of the benchmark are described.

ACRE TFT

Based on information obtained from the developers of the ACRE TFT, the product system was modelled within the software SimaPro. The diagram of the system under assessment is illustrated in Figure 37.

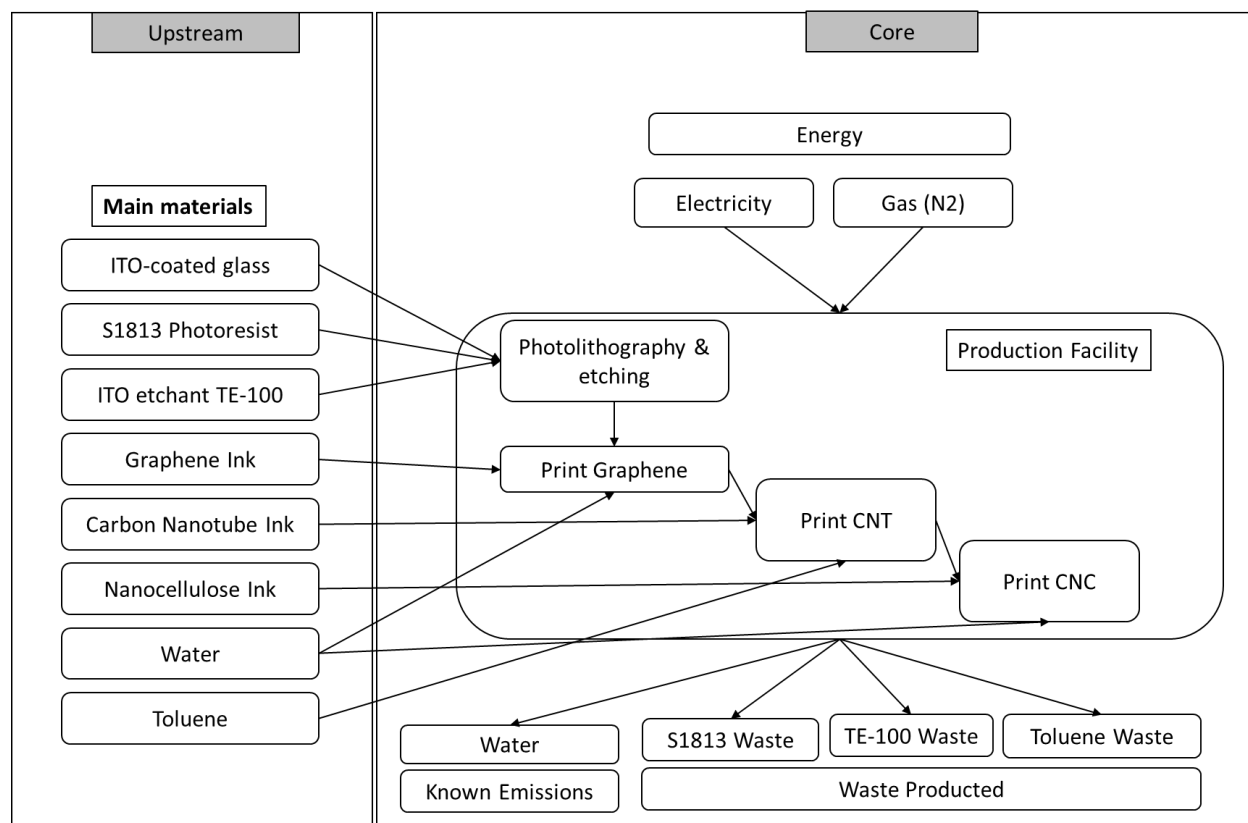


Figure 37 Diagram of the system under assessment divided in Upstream and Core of the ACRE TFT.

In the LCA study, energy and matters flows related to the Upstream and Core of 1 ACRE TFT are considered. As shown in Figure 37, the main materials are purchased and transported to the University developing the ACRE TFTs, where the manufacturing core process of the ACRE TFT takes place.

Benchmark

For the LCA study of the benchmark, the production of a classic transistor is considered. To develop the benchmark, data from the Ecoinvent database served as the primary reference. Since

a cradle-to-gate LCA is carried out, only the process related to the production of a classic transistor is considered.

3.2.3.3. Life cycle inventory

ACRE TFT

For the LCA of the ACRE TFT, primary data was collected in 2023 through questionnaires filled in by the developers of the ACRE TFTs, working at the University. However, since the final product is still in the design phase, some assumptions have been made. Indeed, full data will be available when the MCNM is at higher Technology Readiness Level (TRL). In the production of ACRE TFTs, three distinct types of inks are utilized: one based on carbon nanotubes (CNT), one incorporating graphene, and one using crystalline nanocellulose (CNC). The production of CNTs can be achieved through three methods: Arc discharge, Chemical Vapor Deposition (CVD), and High-Pressure Carbon Monoxide (HiPco). Within the Simapro software, CNTs were modeled using all three methods to create various scenarios. Table 20 provides the sources used for the development of CNTs within the software. For what concerns the other materials used to produce ACRE TFTs (i.e. graphene and CNC), data was collected in 2023 through the above-mentioned questionnaires. However, these data pertained to the production of four identical ACRE TFTs and not just one as identified by the FU. To ensure clarity, the production of ACRE TFTs was analyzed through six scenarios. In one scenario, the input materials collected through the questionnaire, including energy and other resources, were divided by four to assess the impact on a single ACRE TFT. Conversely, another scenario considered the production of one ACRE TFT with material input as one, but using the same amount of energy as required for producing four ACRE TFTs. This approach accounts for the potentially high energy consumption associated with the printer's startup. The exact energy consumption of the machinery between startup and printing operations is unknown, which prompted the creation of various scenarios. These two scenarios help to better understand and estimate the potential energy usage across different phases of operation, ensuring a more comprehensive assessment of the printer's overall impact. Moreover, both scenarios were evaluated for one ACRE transistor with CNTs produced using the Arc, CVD, and HiPco methods, for a total of six scenarios. The scenarios are as follows:

1. 1 ACRE TFT with CNTs ink produced via Arc method;
2. 1 ACRE TFT with CNTs ink produced via CVD method;
3. 1 ACRE TFT with CNTs ink produced via HiPco method;
4. 1 ACRE TFT with CNTs ink produced via Arc method, accounting for higher energy consumption;
5. 1 ACRE TFT with CNTs ink produced via CVD method, accounting for higher energy consumption;
6. 1 ACRE TFT with CNTs ink produced via HiPco method, accounting for higher energy consumption.

In the next paragraphs, LCA-related assumptions along with the processes selected from the databases both for the ACRE TFT and benchmark are reported.

LCA inventory

For the LCA study the assumptions made are the following:

- since only the country of origin of the raw materials was known (e.g. Canada), “market” processes were chosen;
- the carbon nanotubes (CNT) produced by Arc discharge, CVD, and HiPco modelled following (Healy et al., 2008);
- graphene is modelled following (Arvidsson et al., 2014);
- the crystalline nanocellulose (CNC) is modelled following (Li et al., 2013);
- since the processes required to produce the glass substrate for printing the inks were not available in the Ecoinvent database, the process for the glass substrate used to print the transistors was chosen instead.

Table 20 reports all the LCA processes selected from the Ecoinvent database v3.9.1 to model an ACRE TFT.

Table 20 LCA processes from Ecoinvent 3.9.1 database to model the ACRE TFT.

Type	Raw materials	Process name in Ecoinvent 3.9.1 (Cut-off) database
Material	Carbon Nanotubes (Arc/ CVD/ HiPco)	Modelization following (Healy et al., 2008)
Material	Graphene	Modelization following (Arvidsson et al., 2014)
Material	Nanocellulose Ink	Modelization following (Li et al., 2013)
Material	Glass	Glass, for liquid crystal display {GLO} market for glass, for liquid crystal display Cut-off, S
Material	Nitrogen	Nitrogen, via cryogenic air separation, production mix, at plant, gaseous EU-27 S
Material	Toluene	Toluene, liquid {RoW} market for toluene, liquid Cut-off, S
Material	Water to dilute Graphene and CNC ink	Water, decarbonised {US} water production, decarbonised Cut-off, S
Waste	Toluene waste	Spent solvent mixture {RoW} market for spent solvent mixture Cut-off, S
Waste	Water	Wastewater, unpolluted {RoW} market for wastewater, unpolluted Cut-off, S
Energy	Electricity to print ink	Electricity, medium voltage {US} market group for electricity, medium voltage Cut-off, S

Benchmark

For the benchmark LCA study, the Ecoinvent database was used as source of data related to the transistor. *Table 21* reports the LCA process selected from the Ecoinvent database v3.9.1 to model the benchmark.

Table 21 LCA processes from Ecoinvent 3.9.1 database to model the classic transistor.

Type	Raw materials	Process name in Ecoinvent 3.9.1 (Cut-off) database
Material	Transistor	Transistor, wired, small size, through-hole mounting {GLO} market for transistor, wired, small size, through-hole mounting Cut-off, S

3.2.3.4. Life Cycle Impact Assessment

LCA was carried out with the use of the SimaPro LCA software developed by PRé Sustainability. The database Ecoinvent Version 3.9.1 was used for the LCA. ReCiPe 2016 Endpoint and Midpoint methods were used to calculate environmental impacts.

LCA

The following section presents the LCA results for the ACRE TFT compared to the benchmark, a classic transistor. As previously mentioned, the ACRE TFT has been modeled using six different scenarios. These consider different production techniques and energy inputs for creating the transistor with CNTs via Arc, CVD, and HiPco methods. Next to each scenario is the acronym used in both the LCA results showed in Table 22 and Figure 38 Figure 39. The scenarios are as follows:

1. 1 ACRE TFT with CNTs ink produced via Arc method (1 TFT ACRE Arc);
2. 1 ACRE TFT with CNTs ink produced via CVD method (1 TFT ACRE CVD);
3. 1 ACRE TFT with CNTs ink produced via HiPco method (1TFT ACRE HiPco);
4. 1 ACRE TFT with CNTs ink produced via Arc method, accounting for higher energy consumption (1 TFT ACRE Arc en4);
5. 1 ACRE TFT with CNTs ink produced via CVD method, accounting for higher energy consumption (1 TFT ACRE CVD en4);
6. 1 ACRE TFT with CNTs ink produced via HiPco method, accounting for higher energy consumption (1 TFT ACRE HiPco en4).

The results are presented at both the Midpoint and Endpoint levels. Midpoint results are shown in Table 22 as characterized results while Figure 38 illustrates the same results as percentages, with each impact category set to 100%. For each impact category, the most relevant contribution is provided by the benchmark, except for ionizing radiation and fossil resource scarcity. From Figure 38 it is possible to see that for the category of ionizing radiation, the greatest impact is generated by the three TFTs ACRE ("en4"), followed by the benchmark. Similarly, when considering the category of fossil resource scarcity, the three TFTs ACRE ("en4") again account for a substantial portion of the impact due to their energy consumption, followed by the benchmark. In the category of ionizing radiation, the impact percentages are as follows: the three ACRE en4 stand at 100%, the benchmark about 60%, and the other three remaining ACRE at 25%, while in

the category of fossil resource scarcity, the impact percentages are: the three ACRE en4 at 100%, the benchmark at 95%, and the other three remaining ACRE at 65%.

Table 22 Midpoint characterization results of 1 TFT ACRE according to the six assessed scenarios and the classic transistor (benchmark).

Impact category	1 TFT ACRE Arc	1 TFT ACRE Arc en4	1 TFT ACRE CVD	1 TFT ACRE CVD en4	1 TFT ACRE HiPco	1 TFT ACRE HiPco en4	Benchmark	Unit
Global warming	0.056894216	0.09506351	0.057074249	0.095243543	0.056783104	0.094952398	0.147354839	kg CO2 eq
Stratospheric ozone depletion	1.22155E-08	2.96883E-08	1.1988E-08	2.94608E-08	1.19652E-08	2.94379E-08	6.23212E-08	kg CFC11 eq
Ionizing radiation	0.007233315	0.026400058	0.00728989	0.026456634	0.007210336	0.02637708	0.016507139	kBq Co-60 eq
Ozone formation, Human health	8.48719E-05	0.000141853	8.50888E-05	0.00014207	8.4724E-05	0.000141706	0.000496523	kg NOx eq
Fine particulate matter formation	4.98974E-05	9.49426E-05	5.0255E-05	9.53002E-05	4.9659E-05	9.47042E-05	0.000563642	kg PM2.5 eq
Ozone formation, Terrestrial ecosystems	9.10021E-05	0.000150713	9.12328E-05	0.000150944	9.08453E-05	0.000150556	0.000540433	kg NOx eq
Terrestrial acidification	0.000115016	0.000180093	0.000115362	0.000180439	0.000114767	0.000179844	0.001267137	kg SO2 eq
Freshwater eutrophication	1.35792E-05	2.61125E-05	1.36908E-05	2.62241E-05	1.35223E-05	2.60557E-05	0.0001545	kg P eq
Marine eutrophication	9.68287E-07	2.11182E-06	9.74949E-07	2.11848E-06	9.60316E-07	2.10385E-06	8.04175E-06	kg N eq
Terrestrial ecotoxicity	0.186323432	0.237716524	0.186476714	0.237869807	0.186252586	0.237645678	6.259122168	kg 1,4-DCB
Freshwater ecotoxicity	0.002165991	0.003174836	0.002170875	0.00317972	0.002163782	0.003172628	0.07245345	kg 1,4-DCB
Marine ecotoxicity	0.002798243	0.004103484	0.002804678	0.004109919	0.002795294	0.004100535	0.092910084	kg 1,4-DCB
Human carcinogenic toxicity	0.0014124	0.002814497	0.001420456	0.002822553	0.001408443	0.002810541	0.013476563	kg 1,4-DCB
Human non-carcinogenic toxicity	0.03807621	0.061746242	0.038219002	0.061889034	0.038005111	0.061675143	1.252121778	kg 1,4-DCB
Land use	0.001283781	0.00382878	0.001288906	0.003833906	0.001281636	0.003826635	0.004278739	m2a crop eq
Mineral resource scarcity	0.000141507	0.000201251	0.000141528	0.000201273	0.000141208	0.000200952	0.006395711	kg Cu eq
Fossil resource scarcity	0.025729371	0.037699456	0.025777039	0.037747125	0.025694516	0.037664602	0.036786666	kg oil eq
Water consumption	0.00059387	0.000801501	0.000595382	0.000803013	0.000595103	0.000802734	0.001707986	m3

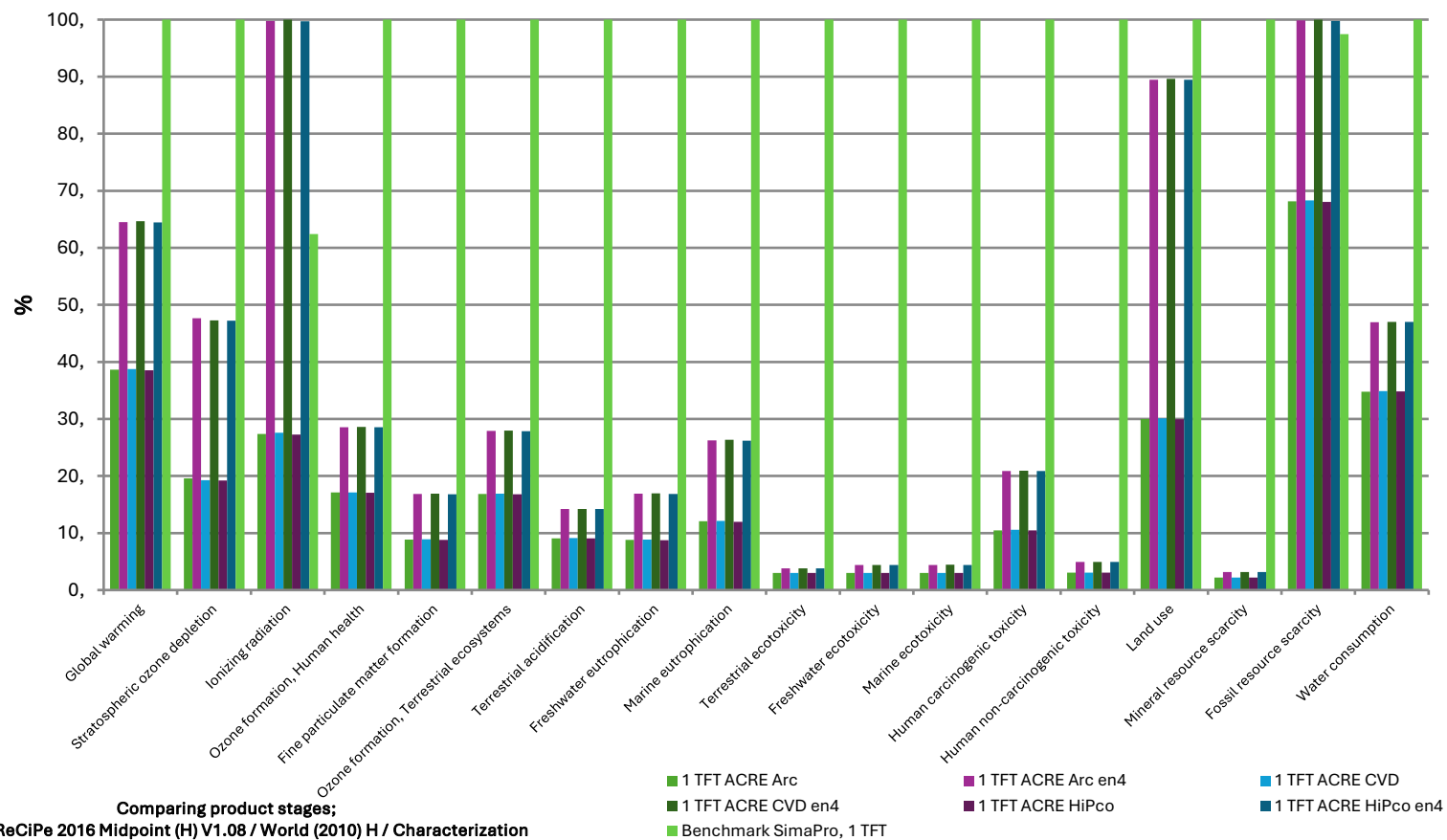


Figure 38 Midpoint characterization results of 1 TFT ACRE according to the six assessed scenarios and the classic transistor.

In general, the data shows that the benchmark or the three ACRE “en4” consistently account for the highest impacts, whereas the baseline ACRE contributes the least. In addition, among the six scenarios, the one with the least impact is the ACRE TFT produced using CNTs made with the HiPco method (Table 22). This finding suggests that the HiPco method offers a more sustainable approach, reducing the overall environmental impact compared to other production methods. This underscores how energy consumption significantly affects the total impact generated by the production of a TFT ACRE. Endpoint results provide an overview of damages to *Human health*, *Ecosystems* and *Resources* caused by the life cycle of both the six scenarios of the TFT ACRE transistors and the benchmark. The normalized results of the three endpoint indicators are reported in Figure 39. Similar to the midpoint results, the largest contributions to the calculated damages for Human Health and Ecosystem categories are related to the benchmark, except for the resource category, where the highest contribution is given by the TFT ACRE 'en4'. Furthermore, the most significant endpoint is the damage to Resources for both the six scenarios of TFT ACREs and the benchmark.

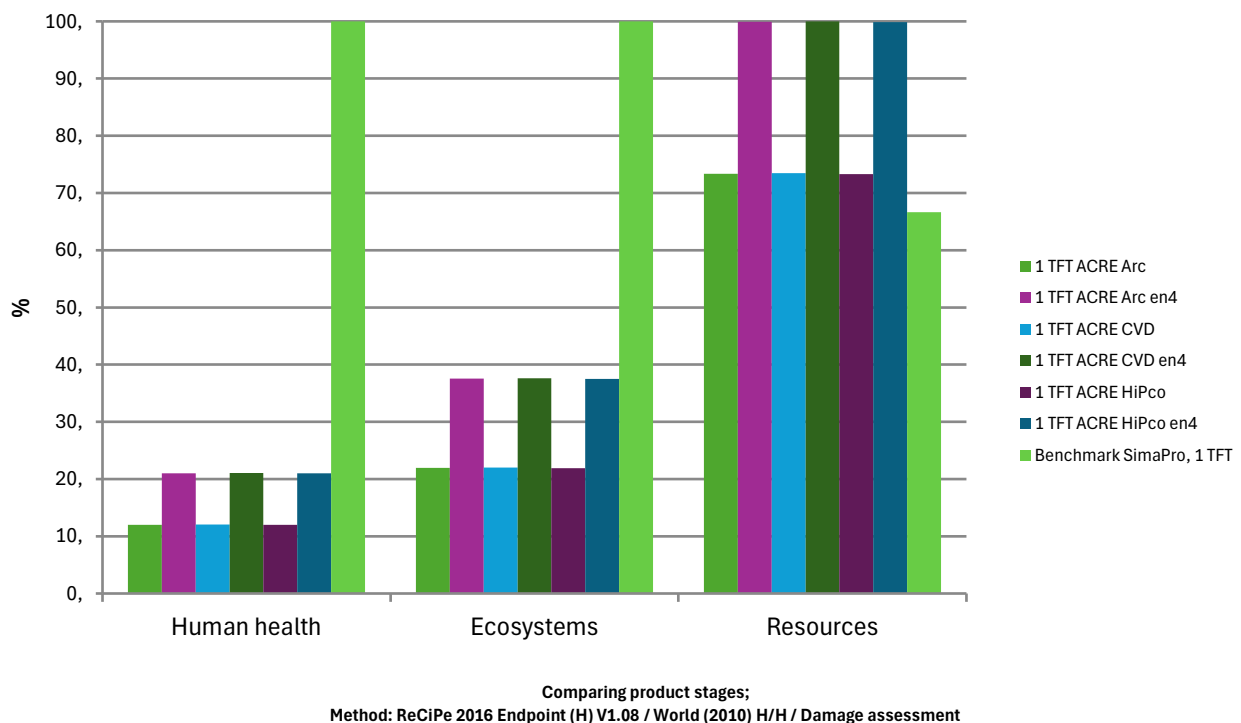


Figure 39 Endpoint results of 1 TFT ACRE according to six scenarios and a classic transistor.

4. Chapter 4 Discussion

This chapter examines and discusses the results derived from the application of Tier 1 and Tier 2 of the developed SUNSHINE SSbD approach to the three case studies, as well as the outcomes of the comparison between SUNSHINE Tier 1 and Early4AdMa Tier 2, all presented in Chapter 3. Specifically, Chapter 4.1 focuses on the results of SUNSHINE Tier 1, Chapter 4.2 analyzes the outcomes of the comparison between SUNSHINE Tier 1 and Early4AdMa Tier 2, and Chapter 4.3 explores the results of SUNSHINE Tier 2.

4.1.Tier 1

Tier 1 methodology has been designed for the early stages of product development. It encompasses a questionnaire which supports the assessment of various aspects associated to safety, sustainability and functionality along the lifecycles of advanced materials. It is a first attempt to derive a qualitative self-assessment procedure to be applied in the R&D stage by industries developing MCNMs to assess the safety, sustainability and functionality performances of their materials/products. Tier 1 is comparative and is designed to support industries, especially SMEs in selecting safer and more sustainable design alternatives for materials/products that are in the early R&D stages of development.

Indeed, the R&D stage is the most relevant in the context of SSbD approaches because, at this stage, safety, sustainability and functionality issues can be addressed and the materials/products being developed can still be modified without incurring excessive costs (Salieri et al., 2021; Tavernaro et al., 2021). In fact, it is during the R&D stage that the potential impacts of the technologies along their lifecycles are investigated and decided. This is thus the stage where the presented Tier 1 questionnaire should be applied using all the available information related to each LCS of the target material/product.

The first part of the questionnaire is an extensive set of general questions for the preliminary evaluation of the target materials/products and the related performances which is needed to properly define the scope and the boundaries of the assessment as well as to accurately evaluate the results provided by the core part of the questionnaire. The latter consists of a set of multiple-choice versatile and intuitive questions which are thought to cover the most relevant aspects to be assessed

and where each provided answer is classified as having positive or negative contributions to safety, sustainability and functionality. This assessment can be applied to assess different alternative solutions and provides a comparison score for each solution by summing up the number of positive contributions for each alternative towards a comprehensive assessment of the target materials/products overall performances.

The added value of this self-assessment methodology was demonstrated through three case studies, (i) PFAS-free anti-sticking coating used on bread baking trays, (ii) active food packaging based on nanodrops of essential oil anchored to the surface of nano clays and encapsulated in a polymeric film as pest barrier, and (iii) all-carbon recyclable electronic (ACRE) thin film transistors (TFTs) used for devices like flat-panel displays. These innovative products were compared with their conventional counterparts (here referred to as benchmark product), Teflon® for the first case study, LDPE for the second and a classic transistor for the latter. The results of this comparison are reported in Figure 4, Figure 5 and Figure 6 for the anti-sticking coating case study and Figure 7, Figure 8 and Figure 9 for the active food packaging case study. The results are not reported for the ACRE TFT case study because, as mentioned in Chapter 3.1, there was no information on the benchmark, and only minimal information on the ACRE TFT from the product developers who filled out the questionnaire. For the anti-sticking coating case study, Figure 4a shows that the baking tray covered with the innovative coating performs better when considering the overall percentage of positive contributions than the one coated with Teflon® for four out of the five assessed life cycle stages. In fact, the EoL stage is the only one in which the anti-sticking coated baked tray has fewer positive contributions than the benchmark. This is due to the fact that, in terms of safety, during the end-of-life life cycle stage, the innovative product has fewer positive contributions compared to the benchmark. There are not available data in literature for emissions on waste Teflon® incineration plants. At lab scale, studies about thermal degradation of Polytetrafluoroethylene (PTFE) (Garcia et al., 2007) showed a very low percentage of semi volatiles, and only very few fluorinated compounds were identified in that group. There are indeed expected emissions for the MCNM-based coating produced by incineration plants. Figure 4b shows the probability that the innovative coating material is better or equal than the benchmark for each life cycle stage. This probability is 100% for the first four life cycle stages, while it is quite low (25%) for the end-of life stage. These results clearly demonstrate that the PFAS-free

anti-sticking coating is superior to the more conventional Teflon® application and therefore it is worthy to continue with its development and possible large-scale production.

The percentage of positive contributions, as previously reported for the life cycle stages, was also estimated for economic, environmental and social sustainability, safety and functionality (cf. Figure 5). Specifically, Figure 5a shows that the MCNM-based coating performs better in all these aspects except for functionality, for which the two alternatives score the same. This demonstrates that the novel coating is competitive with respect to Teflon® because it is safer and more sustainable without compromising functionality. This conclusion is confirmed in Figure 6a, where all positive contributions related to the two compared alternatives are integrated. Figure 6a demonstrates that the innovative material has a higher percentage of positive contributions than the benchmark, while Figure 6b shows that the probability that the innovative material is better or equal than the benchmark is 100%.

Regarding the second case study, Figure 7a shows that the innovative packaging performs better when considering the overall percentage of positive contributions than the LDPE for three out of the five assessed life cycle stages. In fact, the Raw materials and resources stage is the only one in which the innovative material has fewer positive contributions than the benchmark, and for the End-of-Life treatment stage the design alternatives score the same. The benchmark performs better in the Raw materials and resources stage because, among the different aspects, it has more potential positive contribution related to the safety aspect than the innovative material. Figure 7b shows the probability that the innovative packaging material is better or equal than the benchmark for each life cycle stage. This probability is 100% for four life cycle stages, while it is quite low (18%) for the Raw materials and resources stage for the motivation mentioned above. These results demonstrate that the innovative material is superior to the more conventional packaging application and therefore it is worthy to continue with its development and possible large-scale production.

The percentage of positive contributions, as previously reported for the life cycle stages, was also estimated for economic, environmental and social sustainability, safety and functionality (cf. Figure 8). Specifically, Figure 8a shows that the innovative packaging performs better in all these aspects except for Economic sustainability, for which the two alternatives score the same. This is because the answers give for both the innovative material and the benchmark are the same. For social

sustainability and safety aspects, the related uncertainty is quite high, due to the big amount of “I don’t Know” answers, highlighting a gap information. Figure 8b shows the probability that the innovative packaging is better or equal than the benchmark for each life cycle stage. This probability is practically 100% for all the LCS. This conclusion is confirmed in Figure 9a, where all positive contributions related to the two compared alternatives are integrated. Figure 9a demonstrates that the innovative material has a higher percentage of positive contributions than the benchmark, while Figure 9b shows that the probability that the innovative material is better or equal than the benchmark is 100%.

The results provided by the Tier 1 assessment support companies to understand which are the life cycle stages that are weaker in terms of safety, sustainability or functionality performance (i.e. lower percentage) or the assessment results are characterised by high uncertainty. The large number of questions allows evaluation of the assessed aspects from different angles while limiting relevant fluctuations in the case changes are made to the questionnaire, thus leading to solid results. The large number of questions could mean that the questionnaire would be time consuming and require expert input. If this is found to be the case when industrial partners use the tool, simplifications of the questionnaire would be pursued in subsequent versions.

Additionally, it is important to underline that this is a comparative assessment which requires to collect similar information also for the identified alternatives or a benchmark. This applies not only to Tier 1 of the SSbD approach, but also for Tier 2. Nevertheless, as this questionnaire is targeted at users from industry, who are expected to have first-hand information about the technologies they are developing as well as about their alternatives, this should not substantially increase the workload or the level of expertise needed to fill the questionnaire.

It is important to remember that this is a qualitative assessment which can be affected by the subjective opinions of respondents asked to choose among “Yes”, “No”, “I don’t know” and “Not applicable” answers. There are situations where it is difficult to provide a clear answer and situations that require additional clarifications, but the respondent will always choose one of the pre-defined answers, which contributes to uncertainty in the final results. As already explained above, the developed methodology allows to account for these indeterminate results in the comparison of the assessed scenarios. The results of this Tier 1 methodology should always be seen as a first screening

of the assessed materials/products which will be confirmed or denied by the application of Tier 2 assessment.

As a final general consideration, although the questionnaire has been firstly applied to MCNMs, it includes general questions that can be applied, with slight modifications, to a greater range of materials and products, making it applicable to different sectors.

Additional developments of the proposed questionnaire should therefore include a stakeholder consultation process which should also drive the identification of additional questions to cover aspects which are not considered in this version, the derivation of weights to be associated to the provided questions as well as the development of a different integration methodology tailored on the five steps proposed in (Caldeira et al., 2022) and applied in (Caldeira et al., 2023). It is worth noting that the proposed Tier 1 methodology is built on answers which all have the same weights since all questions are supposed to have the same importance. Future developments could be weighted to reflect the different importance of different aspects.

4.1.1. Comparison between SUNSHINE SSbD approach and Early4AdMa approach

In parallel with the developments of the SSbD approach within Sunshine, the Early Awareness and Action System for Advanced Materials (Early4AdMa) approach was simultaneously developed by the OECD. To identify similarities, possible overlaps and complementarities between these two similar approaches, and potential synergies for application by different stakeholders, a comparative analysis was performed. Accordingly, a comparison was made between Tier 1 of the SSbD approach developed in SUNSHINE (ST1) and Tier 2 of Early4AdMa (ET2).

As reported in Table 6 Similarities, differences and complementarities identified comparing ST1 and ET2.” In Chapter 3.1.1, the aspects considered within the two approaches do not completely overlap. ST1 assesses Safety, Environmental, Social and Economic sustainability and Functionality, while ET2 assesses Safety, Environmental sustainability and Applicability to the Regulatory Framework. Additionally, ST1 aims to provide a self-assessment methodology targeted to industries, especially SMEs, while ET2 aims to support companies and regulators towards regulatory preparedness. Moreover, ST1 is comparative, while ET2 is not. It should be noted that in ST1, if for the innovative material there is a potential negative impact related to a specific indicator, such as genotoxicity (considered from the Safety aspect), but a greater number of positive contributions related to other indicators for the Safety aspect in general, then a potentially genotoxic material can be safer than the benchmark, and vice versa. This is because the ST1 doesn’t have alert or red flags for specific questions. Further, for novel materials, there is typically less information available than the benchmark material which could bias the final scoring. ST1 and ET2 questions have been compared as displayed in Figure 11, which points out that, out of all the questions in ST1, 21% are identical, 40% have the same topic, and 39% are not included in the ET2 ones. This means that, summing the percentage of “equal” and “same topic” questions, at least 61% of ST1 questions have something in common with those of ET2. Parallely, ET2 consists of 28% identical questions, 37% that share the same topic, and 35% that are not included in ST1. This means that at least 65% of ET2 questions have something in common with ST1.

The comparison between the results of the application of ST1 and ET2 to the same case study was quite difficult to perform considering that, as reported in Figure 12, only the Safety and Environmental sustainability aspects are in common among the two approaches. Additionally, ST1 presents an overall product performance as reported in Figure 16, while ET2 presents the assessment results divided according to aspects (Figure 17). Accordingly, the comparison among the results from the application of ST1 and ET2 to the same case study could be performed considering only the two aspects that are completely overlapping (i.e. Safety and Environmental sustainability). Within ET2, the results concerning Safety are divided by Human health Safety and Environmental Safety, while ST1 focuses on overall Safety. Consequently, to make the two aspects comparable, the average of the results of Human health Safety and Environmental Safety within ET2 was calculated.

The comparison of the results of ST1 and ET2 applied to the same case study considers that the two approaches express the results in a similar way, but not identically. Indeed, ST1 presents the results as potential positive contributions to a specific aspect, while ET2 presents the results as potential avoided issues to a specific aspect. The comparison has been made between the potential positive contribution (ST1) and the potential avoided issues (ET2) to a specific aspect. For the Safety aspect, ET2 reaches 63% of potential avoided issues while ST1 reaches 62% of positive contributions. As far as Environmental sustainability is concerned, within ST1, the percentage of positive contributions is 71%, while for ET2 the percentage of potential avoided issues is about 70%. These numbers show that the two approaches provide very similar results. A final remark on the application of the results is that within ST1, the uncertainty is calculated using the “I don’t know” answers, while this is not assessed in ET2. Therefore, only the percentage of potential positive contributions and potential avoided issues could be compared between the two approaches.

After investigating the percentage of “equal”, “same topic” and “not considered” questions between the two approaches, the meaning of the answers given for the innovative flame retardant to both questionnaires have been analysed. The focus was on evaluating the significance of the responses rather than the responses themselves due to the contrasting nature of some of the questions posed by the two approaches. For instance, one approach might inquire whether critical materials were used, while the other approach might ask if critical materials were not used. For the questions

considered equal, it has been observed that some responses were different. Indeed, the different responses are likely due to the ST1 questionnaire being completed before the ET2 ones, leading to changes in responses from "I don't know" to "yes" or "no". Then, for questions that share a common topic, the answers can be the same, different, or not evaluable. Some responses are not evaluable because it sometimes occurs that a question in ST1 (or ET2) shares the same topic as multiple questions in ET2 (or ST1). Consequently, there is not a single answer for comparison but multiple ones. Moreover, many questions have different responses between the two approaches precisely because the questions themselves are different. For example, regarding Environmental sustainability, ST1 asks: "Can you reduce water consumption during the production process?". This question was considered to have the same topic, albeit partially, as the following ones in ET2: "Does the manufacturing process, production, transport, use, or consumption require high energy, water, or land consumption or have an impact on global warming potential (emission of greenhouse gases)?" The response given by the innovative flame-retardant case study on the ST1 question was "yes", while it was "no" for ET2, demonstrating that the questions have different responses because the questions are different. Indeed, looking at Table 7, it is evident that only 9% of answers for ST1 questions that overlap in topic with ET2 questions are the same. Similarly, only 12% of answers for ET2 questions with overlapping topics with ST1 questions are the same. Conversely, while ST1 has a higher percentage of "different" answers compared to "not evaluable" answers, ET2 has a higher percentage of "not evaluable" answers. This discrepancy can be attributed to the fact that one question in ET2 covers multiple topics that are addressed by several questions in ST1. As a result, it was not possible to answer many questions in ET2 since a single question encompassed multiple topics from ST1. Finally, the questions defined as not considered indicated which topics are not addressed by the two approaches. Indeed, concerning Safety, ST1 covers a topic that ET2 does not, that of dustiness. For example, ST1 has questions such as: "Does the production process produce dust?" Furthermore, regarding Environmental sustainability, ST1 covered topics that ET2 did not, such as the use of renewable materials, reduction in material consumption, use of renewable energy, reduction in packaging, and use of bio-based packaging. On the other hand, concerning Safety, ET2 covered topics that ST1 did not, such as enhanced properties that may impact risk, changes in the material's kinetic profile, uptake of the material into the body, translocation across barriers, consumer

exposure, use in various products, fate of the material, uptake of the material, and environmental factors as a sink. Finally, regarding Environmental sustainability, ET2 covered a topic that ST1 did not consider, which is the use of raw materials as problematic substances.

On 30th April 2024, the Steering Group on Advanced Materials hosted a Joint SUNSHINE-OECD Workshop to showcase the findings from comparing the ST1 approach with ET2. The session featured presentations on ST1 and ET2 approaches, as well as a detailed comparison between the two. Additionally, the results of applying these methodologies to the innovative flame-retardant case study to further compare the two tools have been shown. Consequently, breakout groups have been created to collect feedback. The main objective of the workshop was to discuss aspects related to the ST1 and ET2 approaches. This included evaluating whether these approaches meet the needs of the intended users, exploring ways to enhance their synergy for better complementarity, and understanding the outlook for motivating potential users to adopt these approaches. The participants in the workshop included researchers (49%), regulators (33%), and industry professionals (18%). They were divided into five discussion groups, with each group intentionally composed of members from all three categories. Each group was asked to answer the following questions:

- Do you think that ST1 and ET2 reflect the needs of the intended users? Do they cover all the relevant aspects?
- What can be done to encourage the application of these approaches?
- Which are the main benefits for a company to apply these approaches?
- Do you think that ST1 and ET2 are complementary or overlapping?

The feedback collected from the participants to the workshop are reported for each question in the following paragraphs.

Question 1: Do you think that ST1 and ET2 reflect the needs of the intended users? Do they cover all the relevant aspects?

Participants stated that both approaches are useful for encouraging thinking on SSbD and even if they differ from the EC Framework, they still evaluate similar aspects. Also, it was confirmed that SUNSHINE approach supports SMEs engaged in developing innovative products. Indeed, due to a SME size, it could be difficult to perform a full SSbD assessment and SUNSHINE really can support them in this, not to mention that SUNSHINE approach can be done without the help of a consultant but internally. Furthermore, it was confirmed that Early4AdMa is useful to monitor early warning and to focus on regulatory preparedness. Moreover, it was stated that both approaches are useful for industries, as they help to identify safety and sustainability concerns in the early stages of innovation, which can lead to the costs reduction. The two approaches could be useful as they bring together all stakeholders in a trusted environment, which can support an early dialogue between innovators and regulators, having an early regulatory advice for innovators thus to anticipate appropriate actions.

On the other hand, participants observed that both approaches address various aspects, but there remains uncertainty about whether all aspects are fully covered. Also, it was mentioned that both approaches lack questions about how life cycle actors engage and how stakeholders are involved throughout the entire life cycle. Specifically, it was noted that SUNSHINE approach has too many questions for companies to use in early stages of development, not to mention that within it all questions are weighted equally which might lead to biased results. Indeed, it has been proposed to add a “warning flag” for those questions which might have a higher weight or if the benchmark is better in the specific question. Regarding Early4AdMa, participants noted that it benefits regulators, but what is considered early for regulators might be late for innovators. Additionally, it was noted that Early4AdMa could benefit from incorporating societal aspects, which are also relevant for regulation.

Question 2: What can be done to encourage the application of these approaches by industries, policy makers and regulators?

To encourage the application of these approaches by industries it was proposed to emphasize that problems are addressed as early in innovation as possible since this is of relevance for business. Also, since the functionality aspect is the most relevant for industry, it is important to highlight that functionality can be connected to safety and sustainability aspects. Furthermore, the importance of

testing the approaches with industrial case studies has been noted. This allows to see how these approaches are applied by people not having a developer or regulator background which further promotes the obtained results and demonstrates the added value and benefits of the applied approaches. However, participants noted that what hampers the use of SSbD approaches is the lack of guidance for using them, the languages in which these approaches are available (currently only the English language is available), and the uncertainty about which are the best tools and approaches available, for a given purpose. Also, it has been specified that it is important that the approaches align with regulatory requirements.

To promote the adoption of these approaches by regulators and policymakers, participants suggested several strategies. They highlighted the need to effectively communicate the benefits associated with using these approaches, e.g. by emphasising the importance to identify opportunities and issues of new materials as early as possible to avoid regrettable decisions. Second, they proposed enhancing the availability of relevant information (e.g. by industry) to allow regulators/decision makers to conclude and not only assume on safety and sustainability and to give feedback to industry. Third, to establish dialogue and discussion with stakeholder on innovation. For encouraging all stakeholders, they recommended organizing webinars, providing training, and offering guidance to stakeholders.

Question 3: Which are the main benefits for a company to apply these approaches?

Participants highlighted that a key advantage for companies lies in gaining insights into the entire value chain. This enables the identification of potential hotspots and the specific life cycle stages in which they occur. Detecting these hotspots early in the development process allows companies to substitute potentially hazardous materials and make informed decisions on the most promising paths for sustainable product development. Additionally, utilizing these approaches can enhance a company's competitiveness. However, participants observed that even if the two approaches are free to use, it takes a long time to fill them out.

Question 4: Do you think that ST1 and ET2 are complementary or overlapping?

Participants emphasized that the two approaches are complementary, even though they partially overlap. Since the two approaches are complementary, they do not need to share the same questions

or operate in the same way. Each approach serves a distinct purpose and is designed for different user groups. The suggestion was made to harmonise questions as far as meaningful but keep the approaches as slim as possible and still acknowledge the different scope and addressees. Given the abundance of available approaches, this integration could lead to a new, more holistic approach. Furthermore, it was suggested to perform further joint case studies by each corresponding addressee to identify differences and whether or not different conclusions will be received as the different users have different information level.

4.2.Tier 2

In this chapter, the Tier 1 results are revisited and integrated with the Tier 2 findings for the selected case studies: a novel PFAS-free anti-sticking coating for the bakery industry, nanodrops of essential oil anchored on the nanoclays encapsulated and incorporated into the polymeric matrix, and an ACRE TFT. The first case study is a nanocomposite coating composed of silica carbide and titanium dioxide (SiC@TiO₂) to be used in bakery industry as a substitute for Perfluoroalkyl and Polyfluoroalkyl Substances (PFAS)-based non-stick coatings, such as Teflon® (Polytetrafluoroethylene or PTFE). The second is composed of nanodrops of essential oil anchored to the surface of nano clays and encapsulated in a polymeric film to be used as a substitute for Low Density Polyethylene (LDPE), produced to develop food packaging that keep the packaged food free of insect pests. Finally, the one to which was partially applied is an All-Carbon Recyclable Electronics (ACRE) thin film transistor (TFT) to replace silicon- or metal oxide-based semiconductor materials.

While Tier 1 qualitative assessment facilitates early identification of potential safety and sustainability ‘hotspots of concern’, Tier 2 provides detailed assessments to support informed decision-making via quantitative CSA and LCSA methodologies, the latter including LCA, LCC, and S-LCA. This structured approach ensures that potential hotspots are identified and addressed during the development process, promoting the creation of safer and more sustainable products. Indeed, while the availability of data and expertise increases in the later product development and optimization stages, they also demand more thorough assessment of safety and sustainability and therefore more comprehensive assessments tools. The operationalization of the tiered SSbD Framework proved that the results and information obtained can support decision-making processes

by discriminating between alternatives in a comparative analysis (i.e., an innovative product compared to a traditional benchmark product).

As mentioned above, the proposed SSbD approach was fully applied to two case studies and partially applied to a third case study. However, in this thesis the application of the CSA foreseen in Tier 2 is not reported as it was not part of the PhD work. Regarding the first case study, Tier 1 application results demonstrated that the baking tray coated with the innovative anti-sticking coating exhibited better performance across various aspects, except for functionality, where both alternatives scored equally. Additionally, the innovative alternative outperforms the benchmark in four out of five assessed life cycle stages, with the end-of-life (EoL) stage being the only exception. This result was further investigated through the application of Tier 2 and, more specifically, of a Life Cycle Sustainability Assessment (LCSA), encompassing LCA, LCC, and S-LCA.

Going into details of the three assessments, the LCA results indicated that the innovative anti-sticking coated baking tray has lower environmental impacts compared to the Teflon®-coated tray. Regarding the LCA, the results for the first four LCSs align with those obtained using Tier 1, whereas the End-of-Life (EoL) scenario is completely reversed. The innovative alternative emerges as the best option by a wide margin. This outcome is largely attributable to the significant environmental impacts associated with the materials, especially the steel used in the tray. Additionally, because the benchmark scenario requires that the tray be discarded annually, this result is to be expected. It is also important to note that this annual disposal aspect was not captured in Tier 1, as the questionnaire posed general questions rather than ones specific to the case studies, meaning some factors may not have been considered.

The LCC, where the benchmark was modelled according to three scenarios (European benchmark, Chinese benchmark, USA-based benchmark), shows results in line with the LCA. In fact, also in this case, it is the cost of materials, and therefore that of steel, that contributes most to the final result. As far as the benchmark is concerned, the results showed that the third scenario (the USA-based) produces the highest economic impacts. The data depicted in Figure 24 highlights the variations in cost distribution across different scenarios, emphasizing the significant impact of transportation and tray costs for the innovative coating compared to traditional benchmarks. This comparison

underscores the necessity of considering geographical and logistical factors when evaluating the overall cost efficiency of materials. It is important to note that Tier 1 does not account for the impact related to the direct cost of materials. This is an aspect that could be considered for a future update to the questionnaire.

Finally, for the S-LCA, the results showed that the innovative material performs better than the benchmark, as also demonstrated by Tier 1. Specifically, the innovative material was compared against a benchmark across three distinct scenarios, each considering the origin of the baked tray: the USA, China, and Europe. Among the benchmarks, the European origin emerged as the most favourable, highlighting the significance of material provenance in conducting a Social Life Cycle Assessment (S-LCA). This finding underscores the critical role that geographic origin plays in shaping the social and environmental impacts associated with material sourcing.

For the active food packaging case study, the Tier 1 application results have shown that the novel packaging provides more positive contributions to both safety and sustainability compared to the benchmark, except for economic sustainability, which is approximately equal for the two alternatives. Such results were observed for all the assessed life cycle stages except for the Raw materials and resources stage, where the benchmark demonstrated higher positive contributions compared to the active food packaging. Also, in this case, the results were further investigated with Tier 2 LCSA.

In Tier 2, the active food packaging was assessed, considering also the environmental benefits of preventing post-harvest food loss. Specifically, in the LCA, it was possible to estimate the environmental impacts that the innovative products can avoid by preventing post-harvest food loss of cereals, which has a world average of 20% (FAO, 2019). In Tier 1, the results show that the benchmark is better than the active food packaging. The distinction between active food packaging and the benchmark lies in the addition of essential oil, which is anchored to a nanoclay embedded within the benchmark. Consequently, even at Tier 2, the impact of active food packaging exceeds that of the benchmark. Looking at the general outcomes, LCA results showed that the benchmark scenarios, both LDPE and biopolymer packaging considered in Tier 2, are the products whose life cycles are associated with higher environmental impacts. Moreover, within this, the downstream phase provides the highest contribution to the environmental impact. In particular, the wheat grain

is the component contributing the most, due to the impacts of the cultivation of grains and the post-harvest food loss. Instead, the active food packaging scenarios (i.e. the LDPE and biopolymer MCNM-functionalized packaging) are less environmentally impactful, having saved 20% of post-harvest food loss.

The Life Cycle Cost (LCC) assessment reveals that the innovative product has significantly lower life cycle costs compared to its respective benchmark. As for the LCA, also for the LCC, the raw materials costs are higher for the innovative product than the benchmark (Figure 34). Figure 33 and Figure 34 highlight that the most impactful cost category for the benchmark is the use phase, particularly due to higher cereal production losses. In contrast, the innovative product demonstrates much lower costs in this phase, suggesting that active food packaging can lead to substantial economic benefits by reducing material losses and improving overall efficiency.

On the social impact front, the Social Life Cycle Assessment (S-LCA) underscores the advantages of active food packaging over the benchmark. As for LCA and LCC, the higher consumption of raw materials for the innovative product compared to the benchmark leads to a higher impact also for the S-LCA. Generally, the results, as depicted in Figure 35, indicate that the innovative product performs better due to reduced food loss and minimized social risks associated with the agricultural sector. Freedom of association and Injuries & Fatalities emerge as the subcategories with the highest medium risk hours equivalent (mrheq). Figure 36 aggregates the subcategories into broader issues, confirming lower impacts for the innovative product in all categories. The most affected category, Health and Safety, aligns with the subcategory-level findings, reinforcing the robustness of the results. Overall, the combined findings from the LCC and S-LCA analyses demonstrate that incorporating the MCNM in packaging solutions not only offers cost savings but also enhances social sustainability. These results underscore the potential of innovative materials to contribute to more sustainable packaging solutions, emphasizing the need for further research and development in this area to fully capitalize on these benefits. The new functionality of the product incorporating the MCNM is crucial to avoid the impacts related to post-harvest food loss. However, it is necessary to stress that the lower impacts are strictly associated with the assumption that the targeted new material users pertain to a context in which post-harvest food loss equals or is higher than the world

average of 20%. It is of utmost importance that the marketization of the active food packaging additive will be directed to countries where the post-harvest food loss is more severe, such as the so-called “developing countries” (FAO, 2021; Kumar & Kalita, 2017; Mesterházy et al., 2020).

Regarding the ACRE case study, the results obtained by the application of Tier 1 demonstrated that the information accessible to the developers of this innovative product was minimal, both for the benchmark and the TFT ACRE. Indeed, Tier 1 can be highly specific, which may create challenges for those tasked with completing it. For example, the questions related to environmental sustainability inquire whether it is possible to reduce water or energy consumption during the production process of a product. Similarly, the questions on social sustainability ask whether suppliers are socially responsible—information that can be difficult for a producer to obtain. In contrast, Tier 2 requires only data on material and energy flows. By leveraging databases such as Ecoinvent and SHDB, it becomes feasible to perform a simplified LCSA (Life Cycle Sustainability Assessment) without needing to complete the questionnaire. In the Tier 2 assessment, a cradle-to-gate Life Cycle Assessment (LCA) was performed. LCA results present a preliminary comparison between the ACRE TFT and the benchmark, a classic transistor, based on six different scenarios. These scenarios encompass varying production techniques and energy inputs for creating the transistor with carbon nanotubes (CNTs) via Arc, CVD, and HiPco methods. Each scenario was analyzed to understand its respective environmental impacts, as indicated in Table 22 and Figure 38 and Figure 39. Midpoint results showed that for most impact categories, the benchmark consistently accounted for the highest impacts, except for ionizing radiation and fossil resource scarcity. In the ionizing radiation category, the greatest impact was generated by the three TFTs ACRE "en4," followed by the benchmark. Similarly, in the category of fossil resource scarcity, the three TFTs ACRE "en4" accounted for a substantial portion of the impact due to higher energy consumption, followed by the benchmark. This indicates that scenarios with higher energy consumption have a more significant environmental impact in these categories. The data highlights that the benchmark or the three ACRE "en4" consistently accounts for the highest impacts, whereas the baseline ACRE contributes the least. This underscores the importance of energy consumption in determining the total impact generated by the production of TFT ACREs. Among the six scenarios, the ACRE TFT produced using CNTs made with the HiPco method exhibited the least environmental impact. This finding suggests that the HiPco

method offers a more sustainable approach, reducing the overall environmental impact compared to other production methods. Endpoint results provided an overview of damages to human health, ecosystems, and resources throughout the life cycle of both the six scenarios of TFT ACRE transistors and the benchmark. The three endpoint indicators revealed that the largest contributions to Human Health and Ecosystem damages were provided by the benchmark. However, in the Resource midpoint, the highest contribution was attributed to the three TFT ACRE “en4.” This indicates that resource depletion is a critical concern in the production of TFT ACREs, regardless of the production method used.

5. Chapter 5 Conclusion

Advanced materials offer significant technological benefits but also pose substantial design challenges, particularly concerning environmental, health, and safety (EHS) issues. These concerns have raised questions not only about the EHS implications of these materials but also about their overall sustainability. This thesis addresses these questions by developing a systematic approach for Safe and Sustainable by Design (SSbD) decision-making for advanced materials like multi-component nanomaterials (MCNMs) and demonstrating it through industrially relevant case studies.

A primary contribution of this research is the development of an SSbD approach to evaluate safety and sustainability along the different stages of advanced materials development, with a specific focus on the early stage of development, where simplified methods are still missing. Following the SSbD Framework proposed by the European Commission, a tiered approach was created to assess safety and sustainability according to the quality and quantity of available data. This approach consists of two tiers. Tier 1 is designed for situations where only qualitative information is available. It consists of a self-assessment methodology that enables industries, especially small and medium-sized enterprises (SMEs), to evaluate safety, functionality, and sustainability in the early design stages. Tier 1 utilizes life cycle thinking, with questions divided based on the life cycle stages of the assessed materials or products. Safety questions are based on risk assessment steps (hazard identification, exposure assessment, and risk characterization) according to EFSA guidance and REACH Regulation. Environmental sustainability questions draw from Life Cycle Assessment (LCA) impact categories (e.g., global warming potential, acidification). Social sustainability questions are inspired by the Social Life Cycle Assessment (S-LCA) methodology, while economic sustainability questions gather information from Life Cycle Costing (LCC). Functionality questions focus on identifying design characteristics that meet customer needs.

Tier 2 is intended for situations where quantitative information is available. It involves comprehensive assessments using the REACH Chemical Safety Assessment (CSA) approach and Life Cycle Sustainability Assessment (LCSA) methodologies, including LCA, LCC, and S-LCA.

The tiered approach allows for different levels of evaluation: when only limited data is available, Tier 1 can be used for a preliminary qualitative assessment. As more detailed data become accessible,

Tier 2 can be employed for thorough quantitative analyses. This ensures that potential EHS risks are identified and mitigated early in the development process, enhancing the overall sustainability and functionality of the products.

In addition, Early4AdMa's Tier 2 (ET2) can be used as complementary tool to SUNSHINE Tier 1 (ST1). This was concluded by a comparison between ST1 and ET2—two SSbD approaches developed simultaneously—that was performed to assist decision-makers in industry, policy, and regulation. The comparison aimed to help select the most suitable methodology to address specific needs and guide follow-up actions. Questions from ST1 and ET2 were classified into common aspects: Safety, Environmental, Economic, and Social Sustainability, Functionality, and Applicability to Regulatory Frameworks. Questions were then compared reciprocally and color-coded: green for equal, orange for similar topics, and red for unrelated. As result, the comparison highlighted that while the two approaches have different goals, scopes, and target different stakeholder groups, they are complementary.

The application of Tier 1 and Tier 2, where, for Tier 2, only the LCSA part was reported, as the CSA was not part of the thesis work but rather the work of other project partners, to a set of case studies (Anti-sticking coated baked tray, Active food packaging and ACRE TFT) allowed for the identification, in addition to strengths, of certain limitations and potential future developments

Among the limitations, those related to Tier 1 are the following: due to its qualitative nature, the evaluation can often be too superficial, failing to provide the depth and detail necessary for well-informed decision-making. This lack of quantitative data means that the reliability of the outcomes may be compromised, making it challenging to draw robust conclusions. Additionally, the generalization inherent in this approach may result in an inadequate capture of the intricacies and complexities of advanced materials. A notable limitation of Tier 1 is that all questions are weighted equally, despite some questions potentially being more problematic or significant than others. This uniform weighting may not adequately reflect the varying degrees of importance or complexity among the questions. Another significant limitation is the substantial number of questions required, which can be time-consuming for companies to complete. Moreover, this extensive questioning often necessitates information that may not be readily available, posing a substantial burden. While the

two case studies conducted within the SUNSHINE project did not encounter issues, the external case study faced considerable difficulties due to these constraints.

The limitations associated with Tier 2 are as follows: this comprehensive quantitative assessment is characterized by its high complexity and the need for specialized expertise. As a result, it becomes difficult for smaller organizations to implement it effectively. Moreover, the process is both time-consuming and costly, which can be prohibitive for certain companies and organizations. A further limitation is the requirement for detailed and specific data, which may not always be readily accessible.

In the future, the developed approach can be significantly improved by designing a preliminary questionnaire with fewer questions than the current Tier 1 questionnaire. This streamlined questionnaire could be applied during the early design phase, allowing companies to provide initial insights without being overwhelmed by the specificity of Tier 1 questions. Once the initial assessment is complete, the detailed questionnaire can be applied. Also, the approach could include "red flags" amongst the list of questions as a basis for "no go" decisions. For example, the question "Does the product incorporating the MCNM release carcinogenic substances during the use phase?" should immediately raise a red flag, thus not contributing to provide a conclusion of the product being "better" than an alternative, as counterbalanced by the "yes" answers to other questions.

As far as the derivation of weights is concerned, the Tier 1 screening level methodology needs to be equipped with an advanced scoring procedure that integrates heterogeneous assessment criteria and indicators with stakeholder trade-offs.

Moreover, the Tier 1 methodology should be better enabled to account for uncertainties in both input data and integration algorithms. Indeed, the proposed approach only accounts for epistemic uncertainties reflected by the "I don't know" answers to the questions. The uncertainties pertaining to the input data that are propagated through the aggregation algorithms into the final results are not considered in the current version. Similarly, the modelling uncertainties stemming from the algorithms themselves are also not estimated.

Additionally, introducing a new Tier between the current Tier 1 (qualitative) and Tier 2 (quantitative) could enhance the process. A semi-quantitative Tier would provide a balanced approach, capturing more detailed insights than qualitative methods while remaining less demanding than full quantitative analyses. By leveraging semi-quantitative methodologies, the evaluation can be both comprehensive and accessible.

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Annex 1

Introduction to the Tier 1 questionnaire

This questionnaire has been developed to support companies producing multicomponent (advanced) nanomaterials (MCNM) in the identification of the main sustainability aspects to be considered when designing materials. The final aims of the Tier 1 questionnaire are to integrate the safety and the sustainability assessment in early stages of the innovation process and to adopt a life cycle thinking approach by considering all the life cycle stages of the innovative product, following the concepts in Figure 1.



Figure 1. Life cycle thinking approach throughout the innovation process.

From a theoretical point of view, sustainable development can be defined as “satisfying the needs of current generations without compromising the ability of future generations to meet their own” (UN World Commission on Environment and Development, 1987). The concept of sustainable development stems from the recognition that the problems of environmental policy cannot be tackled separately from economic and social development. For this reason, sustainable development can be divided into three pillars: Environmental; Economic and Social.

The Tier 1 questionnaire aims at understanding and identifying the possible “SSbD actions” that you might take to improve the sustainability of your product at an early stage of the innovation process.

Annex 2

Table 23 reports the general questions for a preliminary evaluation of the target materials/products

Table 23 General questions for a preliminary evaluation of the target materials/products

	General questions	
N°	MCNM	Product incorporating the MCNM
1	How did you select/identify your innovative MCNM?	
2	Why are you interested in producing your innovative MCNM?	Why are you interested in product containing MCNM?
3	Why combining different NMs is advantageous with respect to applying a single chemical or NM?	
4	Describe your MCNM and its application	
5	Why are you interested in evaluating the sustainability of your MCNM and what benefits could you obtain?	Why are you interested in evaluating the sustainability of your product and what benefits could you obtain?
6	What is the innovative functionality (intended purpose) of your MCNM?	What is the innovative functionality (intended purpose) of your product which is improved by the inclusion of the MC nanomaterial?
7	Which conditions can cause a loss in functionality of the MCNM?	Which conditions can cause a loss in functionality of the product?
8	How do you measure the functionality of your MCNM?	How do you measure the functionality of your product?
9	What is the durability (the ability to remain functional) of your MCNM?	What is the durability (the ability to remain functional) of your product?
10	In which sector can your material be applied (i.e., building sector, energy sector, etc.)?	In which sector is your product applied (i.e., building sector, energy sector, etc.)?
11	Which regulatory Framework(s) related to safety are likely to apply to the MCNM?	Which regulatory Framework(s) related to safety are likely to apply to the final product?
12		What is the minimum amount of MCNM that needs to be incorporated in the product to guarantee functionality?

13	Are the test methods to determine the hazards also adequate for MCNMs?	
14	Is your material developed for an environmentally friendly application (e.g., water purification, renewable energy system, etc.)?	Is your product developed for an environmentally friendly application (e.g., water purification, renewable energy system, etc.)?
15	Can you identify a benchmark [1] material that can be compared with the selected MCNM? Or can you describe the Safe by Design action taken at the material level. Such actions help us in the comparative assessment.	Can you identify a benchmark [1] product that can be compared with the innovative product? Or can you describe the Safe by Design action taken at product level. Such actions help us in the comparative assessment.
16	Which is the scale of application of your MCNM?	Which is the scale of application of the product incorporating the MCNM?
17	At which stage of the innovation process (or on market) is the MCNM?	At which stage of the innovation process (or on market) is the product incorporating the MCNM?

Table 24 reports the request for information for a preliminary evaluation of the sustainability of a MCNM and the related product incorporating the MCNM

Table 24 Request for information for a preliminary evaluation of the sustainability of a MCNM and the related product incorporating the MCNM

N°	Life cycle stage	Please provide the following information	
		MCNM	Product incorporating the MCNM
1	Raw materials/Production	Please provide a flow chart of the MCNM synthesis process, therefore describe the inputs (e.g., chemical input, water input, energy input, etc.) to produce your material (please indicate the related amount of produced product -e.g., 1 mg) and the output (wastes and emissions generated)	Please provide a flow chart of the product synthesis process, therefore describe the inputs (e.g., chemical input, water input, energy input, etc.) to produce your product (please indicate the related amount of produced product -e.g., 1 mg) and the output wastes and emissions generated)
2		Please indicate if you can use a catalyst during the MCNM production process	
3		Please indicate if hazardous degradation products are released during the MCNM production process	Please indicate if hazardous degradation products are released during the product production process
4		Please indicate the yield of your MCNM production process	Please indicate the yield of your product production process

5		Please describe which are the critical quality attributes (physical properties) that drive the functionality of your MCNM (e.g., purity, low impurity levels, physical parameters) and how can the existing process parameters help to achieve these critical quality attributes.	Please describe which are the critical quality attributes (physical properties) that drive the functionality of your product (e.g., purity, low impurity levels, physical parameters) and how can the existing process parameters help to achieve these critical quality attributes
6	Use	Please indicate the potential customers/consumers of your MCNM	Please indicate the potential customers/consumers of your product
7		Please indicate which aspects you consider relevant to improve the sustainability of your MCNM during the use stage	Please indicate which aspects you consider relevant to improve the sustainability of your product during the use stage
8		Please indicate if you can estimate the lifetime of your MCNM	Please indicate if you can estimate the lifetime of your product
9			Please indicate if any transformations (dissolution, aggregation, agglomeration) can be expected during the use phase of the product incorporating the MCNM*
10	End of life (EoL)	Please indicate if your MCNM contains any bio-degradable components	Please indicate if your product contains any bio-degradable components
11		Please indicate which are the recycling/re-use options within a circular economy perspective of your MCNM	Please indicate which are the recycling/re-use options within a circular economy perspective of your product
12		Please describe the alternative EoLs or of similar materials	Please describe the alternative EoLs of your product or of similar products
13		Please indicate if any transformations (dissolution, aggregation, agglomeration) can be expected during the EoL of your MCNM	Please indicate if any transformations (dissolution, aggregation, agglomeration) can be expected during the EoL of your product

Annex 3

The tables below report the case studies answers to the Tier 1 questionnaire along five life cycle stages (LCS): i.e., (1) Raw materials and resources needed to produce the material/product, (2) Production of the MCNM, (3) Production of the product incorporating the MCNM, (4) Use of the product, and (5) End of Life treatment.

Table 25 reports Aspects, Indicators and Questions related to the Raw materials and resources stage along with the case studies answers.

Table 25 Aspects, Indicators and Questions related to the Raw materials and resources stage along with the case studies answers.

Aspects	Indicators	Questions	Anti-sticking coating		Active food packaging	
			Innovative	Benchmark	Innovative	Benchmark
Safety	Chemical components included in authoritative lists	Are any of the chemical components used to produce the MCNM* included in any authoritative lists of restricted and hazardous chemicals (e.g. candidate list of SVHC according to Article 57 of REACH)?	NO	YES	NO	NO
	Carcinogenic raw materials	Are any of the raw materials carcinogenic?	NO	YES	NO	NO
	Genotoxic raw materials	Are any of the raw materials genotoxic (mutagenic)?	NO	YES	NO	NO
	Toxic raw materials	Are any of the raw materials toxic to reproduction?	NO	YES	NO	NO
	Endocrine disrupting properties raw materials	Do any of the raw materials have endocrine disrupting properties relevant to human health?	NO	YES	NO	NO
	Respiratory sensitiser raw materials	Are any of the raw materials a respiratory sensitiser?	YES	YES	YES	NO
	Specific target organ toxicity raw materials	Do any of the raw materials have specific target organ toxicity?	YES	YES	NO	NO

Aspects	Indicators	Questions	Anti-sticking coating		Active food packaging	
			Innovative	Benchmark	Innovative	Benchmark
	Immunotoxic raw materials	Are any of the raw materials immunotoxic?	I don't know	YES	NO	NO
	Neurotoxic raw materials	Are any of the raw materials neurotoxic?	I don't know	YES	NO	NO
	Skin sensitiser raw materials	Are any of the raw materials a skin sensitiser?	YES	YES	YES	NO
	Raw materials that have adverse effects on eye/skin	Do any of the raw materials have adverse effects on eye/skin (e.g. eye damage/irritation, skin corrosion/irritation)?	YES	YES	YES	NO
	Acute toxicants raw materials	Are any of the raw materials acute toxicants?	YES	YES	NO	NO
	Persistent raw materials	Are any of your raw materials persistent, mobile and toxic (PMT) or very persistent and mobile (vPvM)?	NO	YES	NO	NO
	(Acute) ecotoxic raw materials	Are any of the raw materials (acute) toxic to the environment?	I don't know	YES	NO	NO
	(Chronic) ecotoxic raw materials	Are any of the raw materials (chronic) ecotoxic?	I don't know	YES	NO	NO
	Hazardous for the ozone layer raw materials	Are any of the raw materials hazardous for the ozone layer?	NO	YES	NO	NO
	Bioaccumulative raw materials	Are any of your raw materials bioaccumulative?	NO	YES	NO	NO
	Endocrine disrupting properties raw materials	Do any of the raw materials have endocrine disrupting properties relevant to environment?	I don't know	YES	NO	NO
	Physical hazard properties raw materials	Do any of the raw materials have physical hazard properties (explosive, flammable, corrosive, etc.)?	YES	NO	NO	NO

Aspects	Indicators	Questions	Anti-sticking coating		Active food packaging	
			Innovative	Benchmark	Innovative	Benchmark
	Fiber like raw materials	Do any of your raw materials contain fibre like materials (i.e aspect ratio ≥ 3)	NO	NO	NO	NO
Environment sustainability	Critical materials	Are critical materials used? See EU List	YES	YES	NO	NO
	Use of raw materials derived from renewable resources	Do you use renewable raw materials?	NO	NO	NO	NO
Social sustainability	Material resources access	Do your suppliers respect and protect community access to local material resources (i.e., water, land, mineral, and biological resources) and infrastructure (i.e., roads, sanitation facilities, schools, etc.)?	I don't know	I don't know	YES	I don't know
	Health and safety improvement	Does the activity contribute to improvements to (e.g., through sharing health services) the safety and health of the local community?	I don't know	I don't know	I don't know	I don't know
	Health and safety improvement	Does the activity contribute to damage (e.g., use of hazardous materials, pollution) to safety and health of the local community?	NO	YES	I don't know	I don't know
	Traceability of raw materials	Are there policies in place to allow traceability of your raw materials?	NO	NO	YES	YES
	Absence of armed conflicts	Is the origin country of raw materials free from armed conflicts?	I don't know	I don't know	YES	I don't know
	Raw materials coming from underdeveloped, developing or third world countries	Are there restrictive procedures to minimise social issues (e.g., child labour, political or demographic problems, poor working conditions, forced labour, unfair salary, inequality. etc)?	YES	I don't know	I don't know	I don't know
Economic sustainability	Direct costs for raw material	Can you provide the costs of your raw materials?	YES	I don't know	I don't know	YES

Aspects	Indicators	Questions	Anti-sticking coating		Active food packaging	
			Innovative	Benchmark	Innovative	Benchmark
	Direct costs of transportation for raw materials	Can you provide the costs of the transport of your raw materials?	YES	I don't know	YES	YES

Table 26 reports Aspects, Indicators and Questions related to the Production of the MCNM stage along with the case studies answers.

Table 26 Aspects, Indicators and Questions related to the Production of the MCNM stage along with the case studies answers.

Aspects	Indicators	Questions	Anti-sticking coating		Active food packaging	
			Innovative	Benchmark	Innovative	Benchmark
Safety	Chemical components included in authoritative lists	Is the MCNM* in any authoritative lists of restricted and hazardous chemicals (e.g. candidate list of SVHC according to Article 57 of REACH)?	NO	YES	NO	NO
	Carcinogenic MCNMs	Is the MCNM* carcinogenic?	NO	YES	NO	NO
	Genotoxic MCNMs	Is the MCNM* genotoxic (mutagenic)?	NO	YES	NO	NO
	Toxic MCNMs	Is the MCNM* toxic to the reproduction?	NO	YES	NO	NO
	Endocrine disrupting properties MCNMs	Does the MCNM* have endocrine disrupting properties relevant to human health?	NO	YES	NO	NO
	Respiratory sensitiser MCNMs	Is the MCNM* a respiratory sensitiser?	YES	YES	YES	I don't know
	Specific target organ toxicity MCNMs	Does the MCNM* have any specific target organ toxicity?	YES	YES	NO	I don't know
	Immunotoxic MCNMs	Is the MCNM* immunotoxic?	I don't know	YES	NO	I don't know

Aspects	Indicators	Questions	Anti-sticking coating		Active food packaging	
			Innovative	Benchmark	Innovative	Benchmark
	Neurotoxic MCNMs	Is the MCNM* neurotoxic?	I don't know	I don't know	NO	I don't know
	Skin sensitiser MCNMs	Is the MCNM* a skin sensitiser?	I don't know	yes	YES	I don't know
	MCNMs that have adverse effects on eye/skin	Does the MCNM* have adverse effects on the eye/skin (e.g. eye damage/irritation, skin corrosion/irritation)?	YES	YES	YES	I don't know
	Acute toxicants MCNMs	Does the MCNM induce acute toxicity?	YES	YES	NO	I don't know
	Persistent MCNMs	Is the MCNM* persistent, mobile and toxic (PMT) or very persistent and mobile (vPvM)?	NO	YES	NO	I don't know
	(Acute) ecotoxic MCNMs	Does the MCNM* induce any acute environmental toxicity?	I don't know	YES	NO	I don't know
	(Chronic) ecotoxic MCNMs	Does the MCNM* induce any chronic environmental toxicity?	I don't know	YES	NO	I don't know
	Hazardous for the ozone layer MCNMs	Is the MCNM* hazardous to the ozone layer?	I don't know	I don't know	NO	NO
	Bioaccumulative MCNMs	Is the MCNM bioaccumulative?	I don't know	YES	NO	I don't know
	Endocrine disrupting properties MCNMs	Does the MCNM* have endocrine disrupting properties relevant to environment?	I don't know	YES	NO	I don't know
	Physical hazard properties MCNMs	Does the MCNM* have any physical hazard properties (explosive, flammable, corrosive, etc.)?	YES	NO	NO	YES
	Fibre like MCNMs	Is the MCNM* a fibre like materials (i.e high aspect ratio ≥ 3)	NO	NO	YES	I don't know
	Activeroutes of exposure for workers	Are there any active routes of exposure for workers that can be expected during the production of the MCNM*?	NO	YES	YES	I don't know

Aspects	Indicators	Questions	Anti-sticking coating		Active food packaging	
			Innovative	Benchmark	Innovative	Benchmark
	Occupational exposure and upscaled process	Will occupational exposure increase due to the upscaled process?	YES	YES	YES	I don't know
	Chemical or NM emission	Are there any chemical or NM emissions into the indoor environment?	YES	YES	YES	I don't know
	Dustiness from the production process	Does the production process produce dust?	YES	NO	YES	YES
	Liquid emission from the production process	Does the production process cause leaks or releases of liquids?	YES	YES	NO	NO
	NM emissions into the environment	Are there any chemical or NM emissions into the environment? (wastewater and airborne)	YES	YES	NO	YES
Environment sustainability	Critical materials		NO	YES	NO	YES
	Consumption of water resources in production process	Are you in the process of reducing the water consumption during the production process?	NO	NO	YES	NO
	Increase the yield of your process	Are you in the process of increasing the yield of your process?	NO	NO	YES	NO
	Reduce the use of raw materials	Are you in the process of reducing the raw materials use?	YES	NO	YES	NO
	Impact on climate change from production process	Are you in the process of reducing the greenhouse gases when producing your innovative material?	YES	YES	YES	NO
		Are renewable energy resource used?	NO	NO	NO	NO
	Energy consumption during production process	Are you in the process of reducing the energy consumption when producing your innovative material (for instance considering	YES	YES	YES	NO

Aspects	Indicators	Questions	Anti-sticking coating		Active food packaging	
			Innovative	Benchmark	Innovative	Benchmark
		different temperatures and reduce the pressure)?				
	Emissions to water	Are you in the process of reducing the emissions of chemicals and of NM to water generated during the production process?	YES	NO	YES	NO
	Emissions to air	Are you in the process of reducing the emissions of chemicals and of NM to air generated during the production process?	YES	NO	YES	NO
	Waste production during production process	Are you in the process of reducing the waste generated during the production process?	YES	NO	YES	NO
	Reuse of by-product/co-product	Are you in the process of re-use the by-products/co-products generated during the production process?	YES	NO	YES	YES
	Recyclability of waste produced in production process	Are you in the process of recycling the waste produced during the production process?	I don't know	NO	YES	YES
Social sustainability	Health and safety improvement	Does the activity contribute to improvements to the (e.g. through sharing health services) safety and health of the local community?	YES	NO	YES	NO
	Health and safety improvement	Does the activity contribute to damage (e.g. use of hazardous materials, pollution) safety and health of the local community?	NO	NO	NO	NO
	Local employment	Does the organization positively affect the local employment rates?	YES	YES	YES	NO
	Assessment of suppliers	Are suppliers socially responsible (e.g. if they implement CSR principles)?	NO	NO	YES	YES

Aspects	Indicators	Questions	Anti-sticking coating		Active food packaging	
			Innovative	Benchmark	Innovative	Benchmark
	Raw materials coming from underdeveloped, developing or third world countries	Are there restrictive procedures to minimise social issues (e.g., child labour, political or demographic problems, poor working conditions, inequality. etc)?	YES	NO	NO	NO
	Technological development, economic impact, education opportunities	Did you consider if the production process results in technological development, additional education opportunities?	YES	NO	NO	NO
Economic sustainability	Direct costs of waste disposal in production	Can you provide and/or estimate the costs of disposable waste during material production?	YES	NO	YES	YES
	Direct costs of maintenance for production	Can you provide and/or estimate the costs of the material production process?	YES	NO	YES	YES
	Direct costs of installation (heating, lighting) for production	Are installation costs expected for implementing SSbD actions?	YES	NO	YES	NO
	Economic benefits of by-product/co-product	Can you sell your by-product/co-product?	NO	NO	NO	NO
	Direct benefits of production	Can you identify direct economic benefits for the innovative material?	YES	Not applicable	YES	NO

Table 27 reports Aspects, Indicators and Questions related to the Production of the product incorporating the MCNM stage along with the case studies answers.

Table 27 Aspects, Indicators and Questions related to the Production of the product incorporating the MCNM stage along with the case studies answers.

Aspects	Indicators	Questions	Anti-sticking coating		Active food packaging	
			Innovative	Benchmark	Innovative	Benchmark
Safety	Active routes of exposure for workers	Are there any active routes of exposure for workers that can be expected during the production of the product incorporating the MCNM*?	YES	YES	YES	YES
	Occupational exposure and upscaled process	Will the occupational exposure increase due to the upscaled process?	YES	YES	YES	YES
	Chemical or NM emission	Are there any chemical emissions into the indoor environment?	YES	YES	YES	YES
	Dustiness from the production process	Does the production produce dustiness?	NO	YES	YES	YES
	Liquid emission from the production process	Does the production process emit liquid emission?	NO	YES	YES	NO
	Release of bioaccumulating substances	Does your production process release bioaccumulating substances?	NO	YES	YES	YES
	Exposure reduction measures	Do you put in place exposure reduction measures to produce the product incorporating the MCNM*?	YES	YES	YES	NO
	Release of persistent substances	Does your production process release persistent substances?	NO	YES	NO	NO
	Release of carcinogenic substances	Does your production process release carcinogenic substances?	NO	YES	NO	NO
	Release of suspected carcinogenic substances	Does your production process release suspected carcinogenic substances?	NO	YES	NO	NO

Aspects	Indicators	Questions	Anti-sticking coating		Active food packaging	
			Innovative	Benchmark	Innovative	Benchmark
	NM emissions into the environment	Are there any chemical or NM emissions into the environment?	NO	YES	NO	NO
Environment sustainability	Consumption of water resources in manufacturing	Are you in the process of reducing the water consumption during manufacturing?	Not applicable	NO	YES	NO
	Impact on climate change (LCA midpoint) from manufacturing and production process	Do you use renewable energy resource during manufacturing?	I don't know	NO	NO	NO
	Impact on climate change from manufacturing	Are you in the process of reducing the emission of greenhouse gases when designing your innovative product?	YES	Not applicable	YES	YES
	Energy consumption during manufacturing	Are you in the process of reducing energy consumption when designing your innovative product?	YES	Not applicable	YES	NO
	Emissions to water	Are you in the process of reducing emissions of chemicals and of NM to water generated during manufacturing?	YES	NO	YES	NO
	Emissions to air	Are you in the process of reducing emissions of chemicals and of NM to air generated during manufacturing?	YES	NO	YES	NO
	Waste production during manufacturing	Are you in the process of reducing the waste generated during manufacturing?	YES	YES	YES	NO
	Reuse of by-product/co-product	Can you re-use or sell the by-product/co-product generated during the production process?	NO	NO	NO	NO

Aspects	Indicators	Questions	Anti-sticking coating		Active food packaging	
			Innovative	Benchmark	Innovative	Benchmark
	Recyclability of waste produced in manufacturing	Are you in the process of making recyclable the waste produced during the manufacturing be recycled?	I don't know	NO	YES	YES
Social sustainability	Local employment	Does the organization positively affect the local employment rates?	NO	YES	YES	NO
	Assessment of suppliers	Are suppliers socially responsible (e.g., if they implement CSR principles)?	YES	YES	YES	NO
	Raw materials coming from underdeveloped, developing or third world countries	Are there restrictive procedures to minimise social issues (e.g., child labour, political or demographic problems, forced labour, unfair salary, poor working conditions, inequality. etc)?	YES	YES	I don't know	NO
	Technological development, economic impact, education opportunities	Did you consider if the manufacturing process results in technological development, additional education opportunities?	YES	YES	YES	NO
Economic sustainability	Direct costs of waste disposal in manufacturing	Can you provide the costs of disposal of waste during product manufacturing?	YES	NO	YES	YES
	Direct costs of water treatment for manufacturing	Can you provide the costs of water treatment for product manufacturing?	YES	NO	YES	YES
	Direct costs of maintenance for manufacturing	Can you provide the costs of the maintenance for product manufacturing?	YES	NO	YES	YES
	Direct costs of installation (heating, lighting) for manufacturing	Are installation costs expected for implementing SSbD actions?	YES	YES	YES	YES

Aspects	Indicators	Questions	Anti-sticking coating		Active food packaging	
			Innovative	Benchmark	Innovative	Benchmark
	Direct benefits of product	Can you identify direct economic benefits for the innovative product?	YES	Not applicable	YES	YES

Table 28 reports Aspects, Indicators and Questions related to the Use of the product stage along with the case studies answers.

Table 28 Aspects, Indicators and Questions related to the Use of the product stage along with the case studies answers.

Aspects	Indicators	Questions	Anti-sticking coating		Active food packaging	
			Innovative	Benchmark	Innovative	Benchmark
Safety	Release of materials/substances that look like asbestos	Does your product release materials/substances that are fibre like (i.e., aspect ratio ≥ 3)	NO	NO	NO	NO
	Release of persistent substances	Does the product incorporating the MCNM release persistent substances during the use phase?	NO	NO	NO	NO
	Release of carcinogenic substances	Does the product incorporating the MCNM release carcinogenic substances during the use phase?	NO	NO	NO	NO
	Release of suspected carcinogenic substances	Does the product incorporating the MCNM release suspected carcinogenic substances during the use phase?	NO	NO	NO	NO
	Release of bioaccumulating substances	Does the product incorporate the MCNM release bioaccumulating substances during the use phase?	NO	NO	NO	NO
	Chemical or NM emission	Are there any release of MCNM* or of chemical into the environment?	NO	NO	NO	NO

Aspects	Indicators	Questions	Anti-sticking coating		Active food packaging	
			Innovative	Benchmark	Innovative	Benchmark
	Physical hazard properties MCNMs	Does the product have any physical hazard properties (explosive, flammable, corrosive, etc.)?	NO	NO	YES	YES
	Reactivity of the MCNM	Do you expect that the MCNM* could be modified (transformed or degraded) during the use phase?	NO	YES	YES	YES
	Release of MCNM	Do you expect that the MCNM* could be released or dissolved from the matrix during the use stage?	YES	YES	NO	NO
Environment sustainability	Consumption of water resources in product use	Did you consider reducing water consumption when designing the use of your innovative product?	YES	YES	YES	NO
	Impact on climate change from product use	Did you consider reducing the emission of greenhouse gases when designing the use of your innovative product?	YES	YES	YES	NO
	Energy consumption from product use	Did you consider reducing energy consumption when designing the use of your innovative product?	YES	YES	YES	NO
	Emissions to water from product use	Did you consider reducing the emission to water when designing the use of your innovative product?	YES	YES	YES	NO
	Emissions to air from product use	Did you consider reducing the emission to air when designing the use of your innovative product?	YES	YES	YES	NO
	Waste production from product use	Are you in the process of reducing the waste generated during the product use?	YES	NO	YES	YES

Aspects	Indicators	Questions	Anti-sticking coating		Active food packaging	
			Innovative	Benchmark	Innovative	Benchmark
	Less waste, less use of plastic in product use	Are you in the process of reducing the amount of packaging?	YES	NO	NO	NO
	Use of bio-based materials	Can you use bio-based packaging?	I don't know	I don't know	YES	NO
	Repairability of product	Can the product be easily repairable?	YES	YES	NO	NO
	Reuse of chemical substances in product	Can the product be easily reused?	YES	YES	NO	YES
	Recyclability: use of recycled raw materials and production of a recyclable innovative product	Can the product be recycled after use?	YES	YES	NO	YES
		Can the product be dismantled and separated to allow recycling of aspects of the product?	YES	YES	NO	NO
Economic sustainability	Direct benefits of use of product	Are there any direct economic benefits in using the innovative product?	YES	Not applicable	YES	NO
Functionality	Durability	Is the MCNM* designed to have improved durability (the ability to remain functional)?	YES	YES	YES	NO
	Performance	Is the MCNM* designed to have improved performance (the action or process of performing a task or function)?	YES	YES	YES	NO
		Is the MCNM* designed to have an improved incorporating process (easier interaction with matrix, easier applicability, easier processing)?	YES	YES	YES	NO

Aspects	Indicators	Questions	Anti-sticking coating		Active food packaging	
			Innovative	Benchmark	Innovative	Benchmark
	Reliability	Is the MCNM* designed to have an improved reliability (the quality of performing consistently well)?	YES	YES	YES	NO
	Useability	Is the MCNM* designed to have an improved useability (the quality or state of being usable)?	YES	YES	YES	NO
	Versatility	Is the MCNM* designed to be versatile (the quality to be used for different purposes)?	YES	YES	YES	NO
	Customer needs	Have customer needs been mapped?	YES	YES	YES	YES
	Target customer	Did you identify the target customer for the MCNM*?	YES	YES	YES	YES
	Process scalability	Can the design process phase be easily upscaled?	YES	YES	YES	NO
		Can the incorporating process phase be easily upscaled?	YES	YES	YES	NO
	Durability	Is the product incorporating the MCNM* designed to have an improved durability (the ability to remain functional)?	YES	YES	YES	NO
		Do you expect that the MCNM *could be modified during the USE phase (dissolution, release, agglomeration, surface reactivity)?	YES	YES	YES	NO
		Do you expect that the MCNM* surface modifications could affect functionality?	YES	YES	YES	NO

Aspects	Indicators	Questions	Anti-sticking coating		Active food packaging	
			Innovative	Benchmark	Innovative	Benchmark
	Performance	Is the product incorporating the MCNM* designed to have an improved performance (the action or process of performing a task or function)?	YES	YES	YES	NO
	Reliability	Is the product incorporating the MCNM* designed to have an improved reliability (the quality of performing consistently well)?	YES	YES	YES	NO
	Useability	Is the product incorporating the MCNM* designed to have an improved useability (the quality or state of being usable)?	YES	YES	YES	NO
	Versatility	Is the product incorporating the MCNM* versatile (the quality to be used for different purposes)?	YES	YES	YES	NO
	Customer needs	Have customer needs been mapped?	YES	YES	YES	YES
	Target customer	Did you identify the target customer for the product MCNM*?	YES	YES	YES	YES
	Service issues	Can you identify any service issues (e.g., lower performances of the product) related to the product incorporating the MCNM*?	YES	YES	YES	YES

Table 29 reports Aspects, Indicators and Questions related to the End-of-Life stage along with the case studies answers.

Table 29 Aspects, Indicators and Questions related to the End-of-Life stage along with the case studies answers.

Aspects	Indicators	Questions	Anti-sticking coating		Active food packaging	
			Innovative	Benchmark	Innovative	Benchmark
Safety	Worker's exposition	Are workers exposed to MCNM* (i.e., via inhalation)?	NO	NO	NO	NO
	MCNM emission	Are there any expected MCNM *emissions into the environment?	YES	NO	NO	NO
Social sustainability	End-of-life information	Is there clear guidance on the end of life-options provided through labelling?	NO	NO	NO	NO
Economic sustainability	Direct costs of end-of-life	Can you estimate the costs for the end-of-life scenarios of the innovative product?	I don't know	I don't know	YES	YES

Annex 4

Table 30 reports the sources used for the Life Cycle Inventory of the Teflon® coated baking tray system. Indeed, this product system relies entirely on literature data, since primary data were not available.

Table 30 Sources of materials and resources' costs

Material/resource	Cost source
Tetrafluoroethylene	Fluoropolymer Prices, News, Monitor, Analysis & Demand (chemanalyst.com) Polytetrafluoroethylene (PTFE) price index - businessanalytics
Natural gas	www.globalpetrolprices.com/natural_gas_prices
Electricity	www.globalpetrolprices.com/electricity_prices
Transport	20ft and 40ft container: Guide to uses [+ Best prices] (container-xchange.com)
Transport Europe	DELLA™ Transportation prices (rates at transportation, calculation cost transportation, transportation cost, how much transportation price transportation cost and tariffs at transportation, statistics)