SSbD4CheM: Safe and Sustainable by Design framework for the next generation of Chemicals and Materials

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1. Introduction

The Horizon Europe project SSbD4CheM brings together stakeholders from industry, government, academia, and civil society to develop and promote best practices for safe and sustainable product and process design, through demonstration in three case studies. SSbD4CheM aims to meet the EU's strategic objectives for digital, enabling, and emerging technologies, sectors, and value chains. This is achieved through the development of a comprehensive Safe and Sustainable by Design (SSbD) framework, which utilizes new science-based approaches to identify and address potential hazards and risks, along with innovative technologies to support the design of safer and more sustainable products and processes. (Figure 1). SSbD4CheM objectives include:

1) Establishment of a SSbD framework that facilitates development of the next generation of chemicals and materials applicable to renewable composites in automotive value chain, PFAS-free coatings for textile and cellulose nanofibers as additive in cosmetics to replace plastic microbeads,
2) Development of efficient hazard screening tools for alternative assessment of next generation chemicals/materials/products combining *in silico* tools and multicriteria analysis,
3) Advanced explorative ex-ante Life Cycle Assessment (LCA) method supported by molecular and data-driven modelling to fill data gaps for (novel) materials and chemicals,
4) Integration of chemical/(nano-)material characterization methods to assess products' environmental safety and quantify emissions to support occupational and consumer safety limits, and contribute to exposure and risk assessment,
5) Development of alternative, in vitro models, as part of New Approach Methodologies (NAMs) for adequate exposure scenarios,

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6) Harmonization and validation of analytical and toxicological methods for proposition to regulatory and standardization bodies to contribute to the development of new standards and facilitate market acceptance of SSbD4CheM project results, and
7) Enhance overall SSbD4CheM impact through stakeholder engagement, training, dissemination, and exploitation and drive industrial innovation.

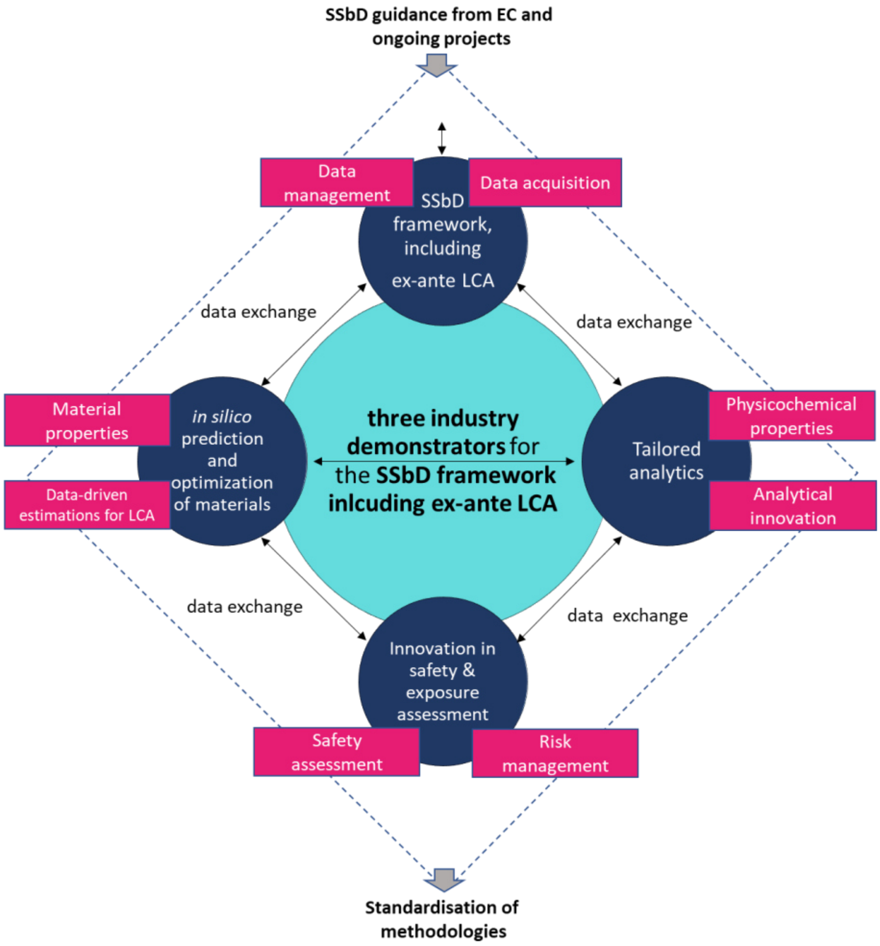

Figure 1: A comprehensive SSbD4CheM toolbox equipped with resources and tools for developing safe and sustainable products and processes.

2. Project Objectives

The strategic goal of SSbD4CheM is to introduce screening and testing methods for safe and sustainable material development in three relevant demonstrators being textile, automotive and cosmetics industry. The demonstrators will be the starting point for further implementation and standardisation of the new methods. The materials/chemicals of the demonstrators include per- and polyfluoroalkyl substances (PFAS) free textile coatings and natural fibres in different composite materials. Screening and testing methods focus on I) physicochemical characterisation with volatile organic compounds, non-uniform particles, and composition of the material, as well as II) risk assessment with exposure and hazard assessment and III) *in silico* prediction tools to reduce experimental delay. For each of the demonstrators an SSbD assessment is performed which will be fed with existing data and newly determined data based on the demonstrators.

3. Case Study 1: Textile

The textile use case's main objective is the experimental development based on the incorporation of bio-based self-cleaning/water repellent and antimicrobial treatments for apparel textiles for the textile market developed by plasma polymerisation and deposition of the coating using the Atmospheric Pressure Plasma (APP). The purpose is to facilitate cleaning and durability of the textile (Polylactic acid yarns, Recycle Polyethylene (PET), virgin PET and their knitted fabrics). These self-cleaning materials will improve the final performance of the apparel textile (Figure 2).

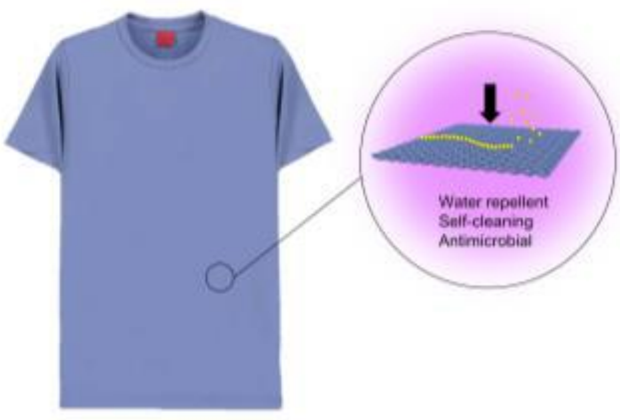

Figure 2: Modification of materials' surfaces for the production of self-cleaning textiles during the SSbD4CheM project.

4. Case Study 2: Automotive

SSbD4CheM project focuses on the renewable composites' formulation development considering recycled polypropylene and polypropylene made from renewable resources as a matrix in combination with micro-fibrillated cellulose and wood fibres as a green alternative for lightweight materials to reduce dependency on oil-based materials and increase materials circularity (Figure 3). Since interior trims are very close and interact with passengers in a relatively close environment, it is important to guarantee they are not an issue in terms of human safety and health. Thus, novel composite materials based on either renewable and/or recycled plastic reinforced by cellulose and wood-based filler will be investigated covering emissions and hazard assessments to enable safe use of such materials from the early R&D phase without any effect on passengers (prototyping).

Figure 3: Automotive interior parts to be modified by renewable composites produced during the SSbD4CheM project.

5. Case Study 3: Cosmetics

Nanocellulose, concretely cellulose nanofibrils (CNF) and cellulose nanocrystals (CNC), a natural material derived from cellulose fibres, has been gaining attention as a potential ingredient in cosmetics to replace plastic microbeads (Figure4). Nanocellulose has unique properties that make it attractive material for cosmetic formulations, including its high surface area-to-volume ratio, ability to absorb and retain moisture, and compatibility with a wide range of other ingredients. One potential benefit of using nanocellulose in cosmetics is its sustainability and biodegradability. As a natural, renewable material, it offers an alternative to synthetic ingredients such as physical peeling, scrub agents, dispersion stabilisers or texture modifiers that may be less environmentally friendly (e.g., plastic microbeads and nylon 6 or 12). However, it is important to note that the production of nanocellulose itself can have environmental impacts, so it's important to consider the entire lifecycle of the material.

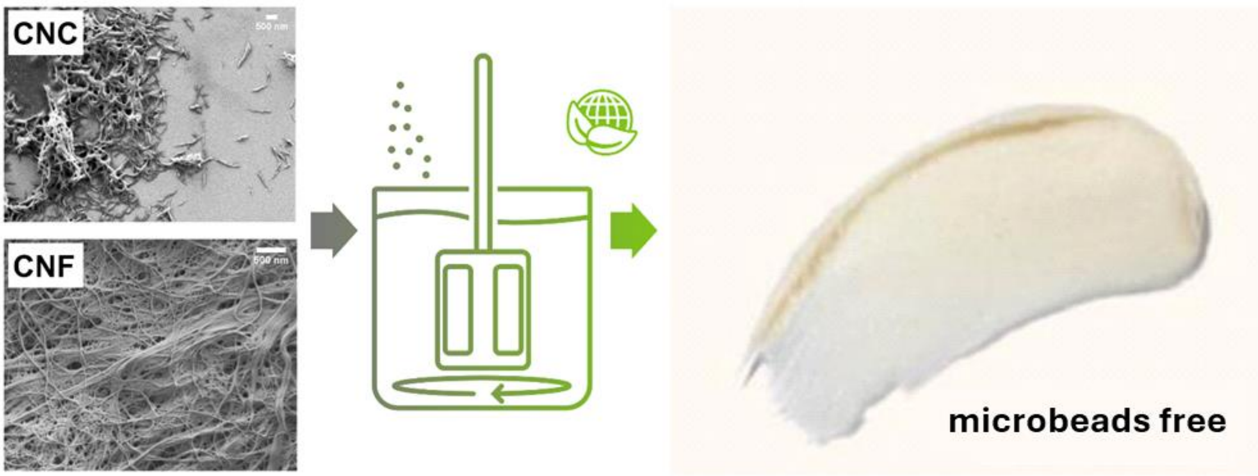

Figure 4: Preparation of cosmetic products using nanocellulose additives (SEM micrographs of CNC and CNF as adopted from [2]) during the SSbD4CheM project.

6. Conclusions

The materials developed within the three different SSbD4CheM case studies will be investigated utilizing computational (e.g., molecular simulations, machine learning, etc.) and advanced analytical techniques (e.g., time-of-flight mass spectrometry, cryo-focused ion beam-ion mass spectrometry advanced imaging, multi-angle light scattering, Scanning electron microscopy with energy dispersive X-ray spectroscopy, Gas Chromatography, Mass Spectrometry). The Safety evaluation methods for human epidermal and dermal topical exposure will be conducted using human skin ex vivo and in vitro models as well as computationally through molecular dynamics simulations. Finally, to guide research and development strategies from the beginning of the material development and ensure environmental competitiveness ex-ante LCA will be performed.

7. References

[1] Grant agreement n° 101138475 (SSbD4CheM)

[2] Oberlintner, A.; Huš, M.; Likozar, B.; Novak, U. *ACS Sustain. Chem. Eng.* **2022**, 10(47), 15480–15489. https://doi.org/10.1021/acssuschemeng.2c04686

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