

FROM THEORY TO PRACTICE: IMPLEMENTING SAFE AND SUSTAINABLE BY DESIGN ACROSS BIO-BASED AND ADVANCED MATERIAL VALUE CHAINS

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BiPhenom



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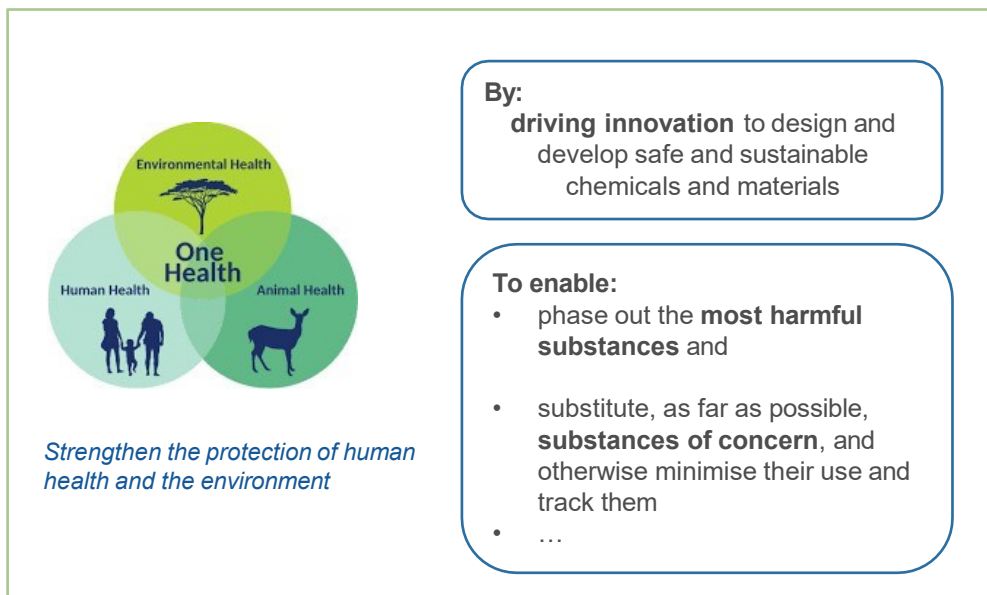
03 From theory to practice – Some of our experiences so far

GREEN DEAL AND CSS

The EU Green Deal



Chemicals Strategy for Sustainability (CSS)



CSS Action Plan

Develop safe and sustainable by design (SSbD) Framework

JRC

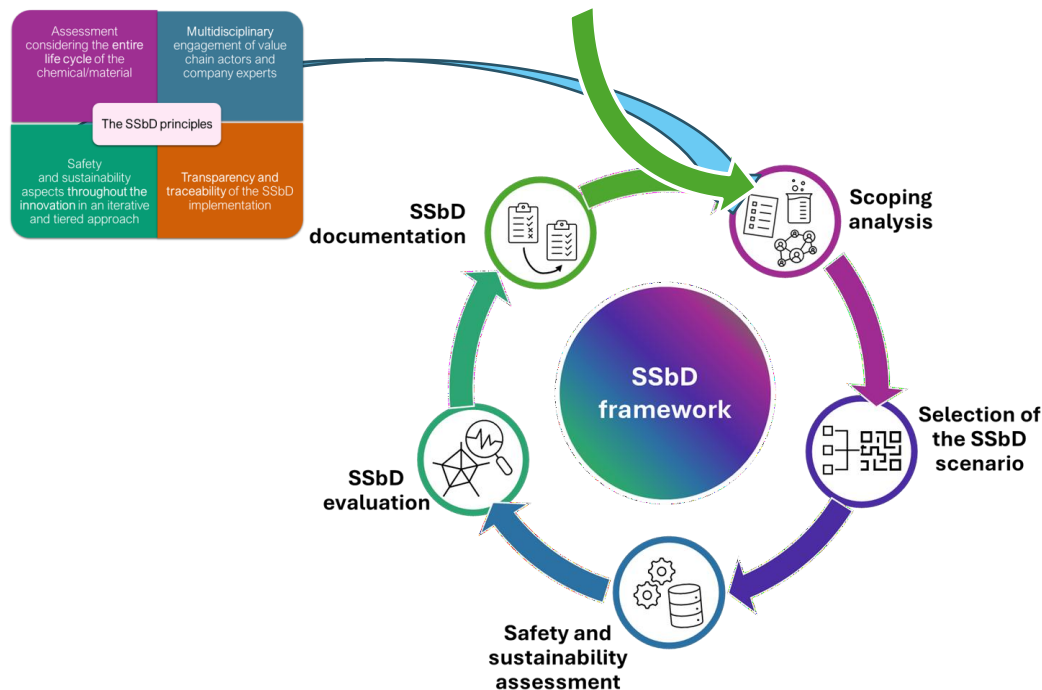


Safe and Sustainable chemicals by design chemicals and materials - Framework for the definition of criteria and evaluation procedure for chemicals and materials. <https://doi.org/10.2760/487955> and <https://data.europa.eu/doi/10.2760/5103785>

Garmendia et al (2025)

SSBD CYCLE: STRENGTHENING INNOVATION WITHIN THE FRAMEWORK

Principles – SSbD cycles – The SSbD System



The SSbD System

What is the chemical/material life cycle in which the innovation is happening?

The innovation

The goal

Why is the innovation happening? What is the goal?

(re)design action

What is the innovation (breakthrough or incremental) applied to achieve this goal? **Where** is it taking place? Molecular, process, product?

Indicators and decision rules

How is the success of the innovation proved? **What** are the aspects and indicators that will demonstrate that the goal has been achieved applying the (re)design?

Maturity of innovation/Maturity of SSbD

When is the SSbD implemented?

Actors in the life cycle

Who are the actors in the life cycle involved in the innovation/SSbD implementation? **What** are their responsibilities and needs in the innovation with regards to the safety and sustainability performance?

Documentation

How has the implementation of the SSbD been done?

LIST AND SSbD

Environmental Sustainability Assessment and Circularity (SUSTAIN Unit)

Three LIST groups:

- Environmental Policies (EPS)
- **Environmental Health (EH)**
- Life Cycle Sustainability Assessment (LCSA)

LIST activities related to

- Preliminary assessments of safety – environmental sustainability – policy recommendations
- **Safety** – Safety screening, hazard assessment, NAMs / *in vitro* toxicology, toxicity and eco-toxicity testing
- **Sustainability** – Life Cycle Assessment, indicators, Social LCA, sustainability criteria

Projects

- CHIASMA - *in vitro* and *in silico* methods, NAMs for SSbD
- INSIGHT / PINK (sister projects of CHIASMA) – Integrated impact assessment and Computational models for SSbD
- ZeroF – bio-based coatings to replace PFAS (textile/packaging)
- SuperBark – bio-based adhesives and coatings from bark (packaging/wood)
- BioPhenom – functional biophenols (thermosets, impregnated wood, bio-composites)
- DESIDERATA – SSbD alternatives for metalworking, construction, injection moulding and 3D printing)



SCOPING THE INNOVATION - THE OFTEN-OVERLOOKED FIRST STEP

What scoping delivers

Common technical and terminological basis

- across chemists, material scientists, LCA experts, economists, data engineers, SSbD practitioners

Defined system boundaries and functional units

- 1 m² coated product, 1 kg of lubricant, reference scenarios (PFAS or SoC)

Identified design alternatives and data requirements per value chain

- Standardised data collection templates - supporting FAIR data principles and reducing workload across partners.

Mitigated risk of fragmented objectives in large consortia

Highly appreciated even without formal status in the 2022 framework - formalised in the December 2025 revision

Project / UC	Functional Unit
ZeroF Packaging	1 m ² coated paper
ZeroF Textiles	1 m ² coated fabric
SuperBark Wood	1 m ³ finished wood product
SuperBark Paper	1 m ² coated paper
DESIDERATA UC1	1 L formulated lubricant
DESIDERATA UC2/3	1 kg compounded pellets
DESIDERATA UC5	1 m ² / 1 m ³ insulation panel

GREEN DESIGN PRINCIPLES - FROM ASPIRATION TO TECHNICAL INDICATORS

Eight (re)-design principles

P1 - Material Efficiency / P2 - Minimise Hazardous Chemicals / P3 - Energy Efficiency

P4 - Renewable Sources / P5 - Prevent Emissions / P6 - Reduce Exposure

P7 - Design for End-of-Life / P8 - Whole Life Cycle

- ZeroF (P2 & P6): 20+ substances substituted, prioritised, or reduced. Adapted lab techniques/ methodologies minimised resource use and process emissions.
- ZeroF (P4): Bio-based CeFAE (cellulose + fatty acids) replaces fossil-based PFAS → drives major LCA improvements.
- DESIDERATA (P2+P6): UC1 graphene at 1-5% replaces MCCP/LCCP at 70% of lubricant. UC5 bio-based surfactants eliminate hazardous Alum powder and H₂ gas generation. UC3/UC4: PTFE substitution eliminates a key PFAS from additive manufacturing and industrial coatings.
- Design principles have a guidance role only, not sufficient to label a material as "SSbD".

HAZARD SCREENING - MAKING SAFETY A PRIMARY DESIGN DRIVER

Safety initial activity - Hazard Classification (26 endpoints, CLP-aligned)

- H1 - Most Harmful / SVHC - Score 0 - FAIL (Cut-off, substitute)
- H2 - Substance of Concern - Score 1 - Pass* (Minimise)
- H3 - Other Hazard - Score 2 - Pass (Monitor)
- H4 - No H1-H3 - Score 3 - Pass (Proceed)

ECHA, OECD eChemPortal, QSAR Toolbox + automated *in silico*

ZeroF products / Name	Physical form	SSbD hazard class	SSbD score	Unresolved data gaps for H1 classification
Powder 1 and 2	Powder	4	3	Carcinogen, Mutagen, Reproductive toxicity, Respiratory sensitiser, ED, STOT RE, PBT
P1-P2-P3 basis formulation	Liquid	2	1	Gaps for polymers and polymeric networks, mixture classifications
P4 formulation	Liquid	2	3	Gaps for polymers and polymeric networks, mixture classifications

HAZARD SCREENING - MAKING SAFETY A PRIMARY DESIGN DRIVER

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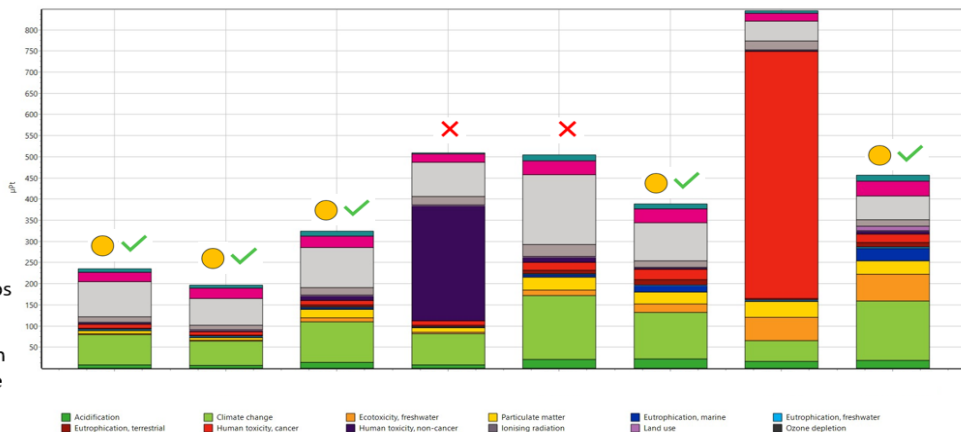
- Across all projects: hazard screening is one of the most impactful early SSbD activities - preventing regrettable substitution before synthesis commitments are made.

Safety screening – recommendation ;

✗ No go*

● Data gaps

✓ Okay based on available data



	Environmental Hazards						
	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Ozonelayer	PBT/vPvB	PMT/vPvM	Endocrine disruption (environment)	Data source
Alternative 1	MISS	3	MISS	MISS	MISS	MISS	REACH Joint
	NC	NC	NC	NC	NC	NC	CLP Submission
	NC	NC	NC	NC	NC	NC	CLP Submission
							Not registered in ECHA Database
	NC	NC	NC	NC	NC	NC	REACH Joint
	NC	NC	NC	NC	NC	NC	CLP Submission
	MISS	MISS	MISS	MISS	MISS	MISS	CLP Annex VI
	MISS	4	MISS	MISS	MISS	MISS	CLP Submission
	NC	NC	NC	NC	NC	NC	CLP Submission
	NC	NC	NC	NC	NC	NC	REACH Joint
Alternative 2	MISS	3	MISS	MISS	MISS	MISS	REACH Joint
	NC	NC	NC	NC	NC	NC	CLP Submission
							Not registered in ECHA Database
	NC	NC	NC	NC	NC	NC	REACH Joint
	NC	NC	NC	NC	NC	NC	CLP Submission
	MISS	2	MISS	MISS	MISS	MISS	CLP Submission
	MISS	MISS	MISS	MISS	MISS	MISS	CLP Annex VI
	MISS	4	MISS	MISS	MISS	MISS	CLP Submission
	NC	NC	NC	NC	NC	NC	CLP Submission
	NC	NC	NC	NC	NC	NC	REACH Joint
Alternative 3	MISS	2	MISS	MISS	MISS	MISS	CLP Submission
	MISS	3	MISS	MISS	MISS	MISS	REACH Joint
	NC	NC	NC	NC	NC	NC	REACH Joint
	NC	NC	NC	NC	NC	NC	CLP Submission
	NC	NC	NC	NC	NC	NC	CLP Submission

IN SILICO METHODS & NEW APPROACH METHODOLOGIES

Gap-filling strategies

1. Existing public data - ECHA, eChemPortal, SDS, literature

2. In silico predictions - QSAR, conformal prediction, read-across

- e.g., polymer structures and properties

3. In vitro (NAMs) - ALIsens® air-liquid interface (LIST)

- Inhalation toxicity, sensitisation markers

QSAR models fall outside applicability domains for novel polymers and polymeric networks.

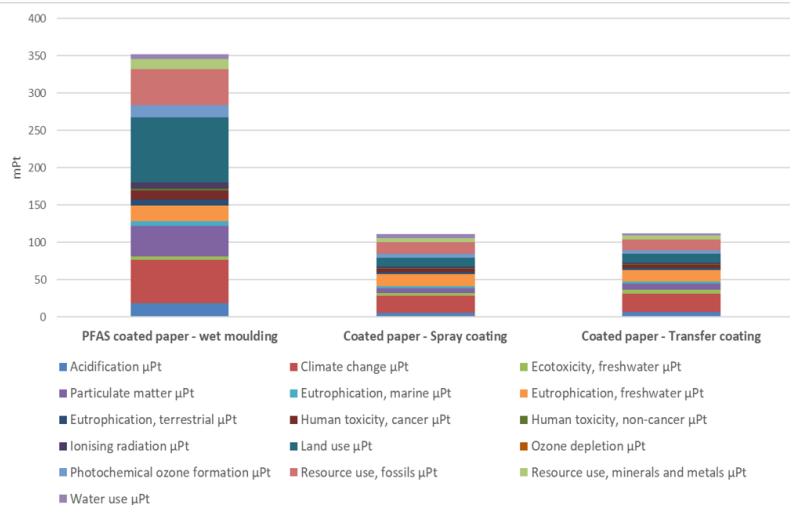
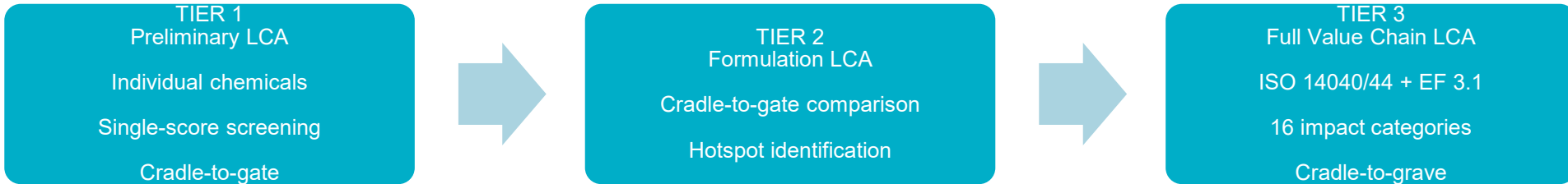
Critical endpoints (ED, carcinogenicity): OECD *in vitro* tests are recommended (TG 301/310, TG 305, TG 201–203).

Route	TIER 1	TIER 2	TIER 3
Inhalation	SDS + in silico	A549/Calu-3	MucilAir™/AlveolAir™, AOPs
Dermal		HaCaT monoculture	OECD TG 431/439 · AOP
Gastrointestinal		HepG2/Caco-2	EpilIntestinal™ triculture
Others		ED (TG 455), Neurotoxicity (NAMs) CTA	[In silico] RNA+DNA sequencing; AOPs

Formalise the empirical application: a structured three-tier testing strategy explicitly linked to life cycle stages

TIERED LCA FOR ENVIRONMENTAL SUSTAINABILITY

Cross-project lesson: Tiered LCA starting early, even with incomplete data. Provides directional guidance for formulation choices and prevents costly late-stage redesign.



LCA Assessment level	Impact category	Unit	Impact PFAS	Impact Powder	% change	Score	Level
Toxicity	Human toxicity, cancer effects	CTUh	1.14E+01	4.22	68%	3	Pass
	Human toxicity, non-cancer effects	CTUh	3.08	1.34	61%	3	
	Ecotoxicity freshwater	CTUe	4.79	2.99	38%	3	
Climate change	Climate change	Kg CO ₂ eq	58.42	22.84	84%	3	Pass
Pollution	Ozone depletion	Kg CFC11eq	5.46E-02	0.017	55%	3	Pass
	Particulate matter	Disease inc.	4.06E+01	6.51E+00	21%	3	
	Ionising radiation	kBq U-235 eq	8.38	1.99	67%	3	
	Photochemical ozone formation	kg NMVOC eq	15.87	4.90	63%	3	
	Acidification	mol H+ eq	18.084	5.799	56%	3	
	Eutrophication, terrestrial	mol N eq	8.86	2.96	76%	3	
	Eutrophication, freshwater	kg P eq	20.60	16.24	86%	3	
	Eutrophication, marine	kg N eq	6.21	2.79	69%	3	
	Land use	Pt	87.085948	11.846616	86%	3	
Resources	Water use	m3 depriv.	6.9122348	4.6094349	33%	3	Pass
	Resource use, minerals and metals	kg Sb eq	13.053498	5.4528998	58%	3	
	Resource use, energy carriers	MJ	48.74031	16.028008	67%	3	

PARALLEL ASSESSMENT - SAFETY + SUSTAINABILITY + SOCIO-ECONOMICS

Integration - Two-way aggregation

- Consideration of functionality, safety, sustainability, socio-economic aspects
- Requires knowledge on Operational Research (e.g., MCDA)

- JRC integration of Safety/Sustainability →

		Environmental score			
		0	1	2	3
Safety score	4	L1	L2	L3	L4
	3	L1	L2	L3	L3
	2	L1	L2	L2	L2
	1	L1	L1	L1	L1
	0	L0	L0	L0	L0

- Example of LCC results
- LCC = decision-support tool, not pass/fail at low TRL. Cost at material level ≠ end-user product cost increase.

Material	Cost	vs PFAS	Score
Powder 1	€0.379/m ²	+24%	0
Coating P1	€43.5/kg	-16%	3
Coating P4	€58.9/kg	+13%	1

LOW TRL ENVIRONMENTS & DATA GAPS - NAVIGATING UNCERTAINTY

- **Design alternatives** not excluded based on SSbD results alone, given expected data uncertainty
- **Speed mismatch:** Innovation cycles may move faster than complex safety assessments. Safety data may arrive *after* design decisions are already made.
- **In silico applicability limits:** models outside applicability domains for complex materials. Are predictions (un)reliable?
- **Commercial product "black boxes":** Commercial materials may contain SoC, are SDS sufficient? No standardised way to incorporate in SSbD at the moment.
- Framework requires an extremely **high level of expertise, resources** and communication effectiveness, often **exceeding the capacity** of standard innovation departments → key barrier to broader industrial adoption

RECOMMENDATIONS - BRIDGING THEORY AND PRACTICE

Strategic goal: Transition SSbD from a "research-intensive exercise" to a standard industrial practice - applicable within realistic resource constraints, with standardised methods, validated tools, and a connected data ecosystem

01 - TIERED, TRL-ALIGNED ASSESSMENTS

- Low TRL: molecular design hypotheses + initial hazard screening with "acceptable uncertainty" - on pre-defined timelines
- High TRL: full-scale LCA and socio-economic studies when composition stabilised
- Use SSbDL maturity framework to structure early scoping

04 - TRUSTED ENVIRONMENT & VALUE CHAIN ENGAGEMENT

- Ensure a Trusted (innovation) Environment: secure SSbD data exchange among all, preserving IP rights.
- Multi-actor cooperation essential
- Stakeholder engagement accelerates results/framework adoption



02 - FAIR DATA & STANDARDISED TEMPLATES

- Harmonised data collection templates
- FAIR data principles (Findable, Accessible, Interoperable, Reusable) essential for long-term reliability
- FAIRification reduces workload and enables cross-comparison

03 - TOOL VALIDATION & STAGE-GATES

- Validation paths for in silico tools (enhance decision applicability)
- Define stage-gates for SSbD decisions - open-ended decision spaces reduce convergence
- Exposure-based risk approach (revised framework)

SSbD can work: With multidisciplinary collaboration, FAIR data infrastructures, validated tools, stage-gate decision processes, and Trusted Environments for efficient data exchange. From a research methodology, to an industrial and regulatory necessity

thank you

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