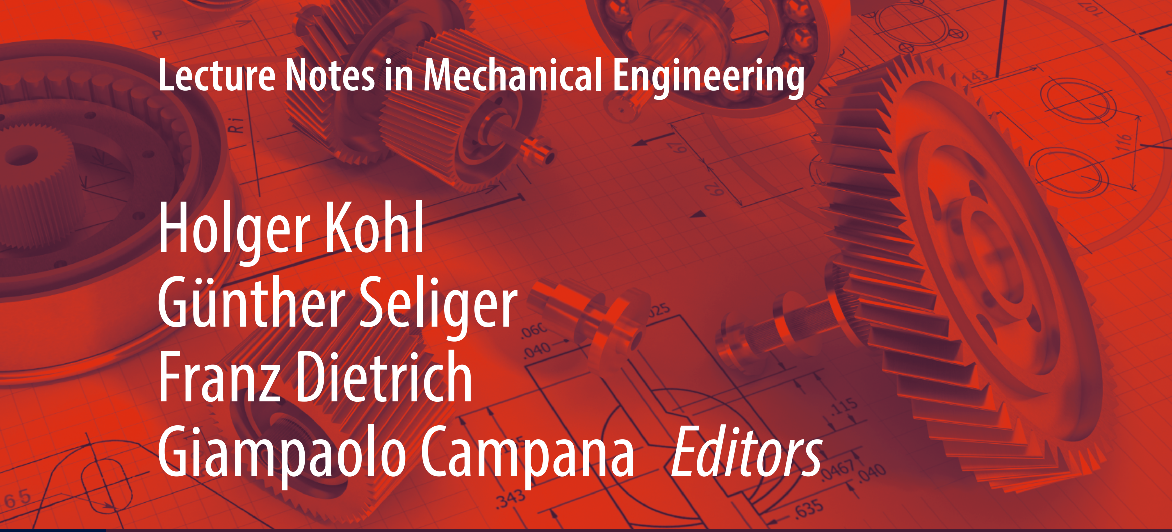

Lecture Notes in Mechanical Engineering

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Safe and Sustainable Value Creation by Design

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Towards Addressing Co-Creation Gaps: Automating Safe-and-Sustainable-by-Design Workflows with Electronic Lab Notebooks

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Abstract. The Safe-and-Sustainable-by-Design concept integrates Safety Assessment and Life Cycle Assessment tools to create a new systematic approach addressing challenges in chemical safety, environmental impacts, and material circularity. However, fragmented data sources, complex assessments, and a lack of efficient collaborative tools hinder its effective implementation. This work outlines a structured, co-creative approach to the Safe-and-Sustainable-by-Design process, leveraging automated workflows to overcome these challenges.

A central component is an Electronic Lab Notebook configured to represent essential Safe-and-Sustainable-by-Design resources - chemicals, materials, (manufacturing) processes, and products/applications - while serving as a structured repository for laboratory experiments, hazard assessments, production safety, and environmental sustainability evaluations. These elements are integrated into a Safe-and-Sustainable-by-Design innovation and (re)design stage-gate workflow.

With programmatic Application Programming Interface access, the Electronic Lab Notebook supports automated workflows, including material property prediction, structured and unstructured data retrieval from chemical and material databases, and integration with external assessment tools. Team members can add materials via a web interface, associate them with Safe-and-Sustainable-by-Design stages, and trigger automated assessments or data gap-filling.

This modular approach allows a seamless mix of manual and automated assessments while ensuring structured documentation, organization, and traceability. Unlike ad-hoc file-sharing, we expect Electronic Lab Notebook to foster real-time collaboration, helping decision-making through well-documented iterative Safe-and-Sustainable-by-Design workflows.

Keywords: Safe-and-Sustainable-by-Design · Electronic Lab Notebook · Data Management

1 Introduction

Safe and Sustainable by Design (SSbD) is a voluntary framework promoted by the European Commission to guide the development of chemicals and materials toward sustainability goals. It aims to minimize health and environmental impacts across the

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lifecycle - from sourcing and production to use and end-of-life - while steering innovation away from substances of concern. SSbD is structured as an iterative process combining a (re-)design phase, guided by sustainability principles, with a multi-criteria assessment phase covering hazard, exposure, and life-cycle considerations.

Recent consultations with the SSbD stakeholder community have identified several key gaps limiting effective uptake [1]:

Data generation gaps: The need to develop and apply New Approach Methodologies (NAMs) to address chronic endpoints, degradation of mixtures, and Adverse Outcome Pathways (AOP)-based justification; and to develop and validate AI methods to support prediction and screening in SSbD;

Methodological framework gaps: Shortcomings in current Life Cycle Assessment and Product Environmental Footprint methodologies;

Co-creation and usability gaps: A key challenge is to test, adapt, and *co-create SSbD assessment methods* that support decision-making during the sustainability transition in the chemical sector. In parallel, there is a need to develop a better understanding of socio-economic factors that influence interactions between chemicals and people. Another critical gap concerns the education, training and skills.

SSbD community networks are being established (https://iriss-ssbd.eu/), and decision support tools are being developed – e.g. PARC SSbD Toolbox (https://www.parc-ssbd.eu/), HARMLESS Decision Support System with AMEA (Advanced Material Earliest Assessment), WASP (Warning flags, design Advice & Screening Priorities), and ASDI (Alternative SSbD Design Inspector) tools. However, still there are a lack of *concrete and usable tools that support day-to-day collaboration among diverse actors*. Specifically, what is lacking includes:

- Shared digital environments where experts and stakeholders can collaboratively evaluate materials and processes based on *evolving* evidence.
- Interoperable data formats and structured workflows, to translate experimental results, expert judgments, and model outputs into traceable, reproducible, and decision-relevant documentation and enable transparent linkage between evidence and decision versus existing practice scattered reports and spreadsheets.
- Mechanisms for iterative feedback and versioning, to allow stakeholders to revisit and revise prior decisions as new data or criteria become available.
- Automation and Application Programming Interface (API) accessibility, to connect manual and computational assessments, reducing delays and human error in complex, multi-stage evaluations.

SSbD is fundamentally a collaborative, multidisciplinary process. Chemists, toxicologists, materials scientists, engineers, and sustainability experts must work together across different stages - synthesis, characterization, assessment, and selection. While shared folders are commonly used to collaborate, they fall short when it comes to supporting the kind of structured, transparent, and iterative work that SSbD requires. Files are often scattered or inconsistently named, and it is difficult to trace what data informed a particular choice or how to update that choice when new data arrives. This is especially problematic in SSbD, where teams with different expertise must work together and contribute data at different stages. Misunderstandings, duplicated work, and missed insights can be avoided with a shared structure and rules for how information is recorded and connected.

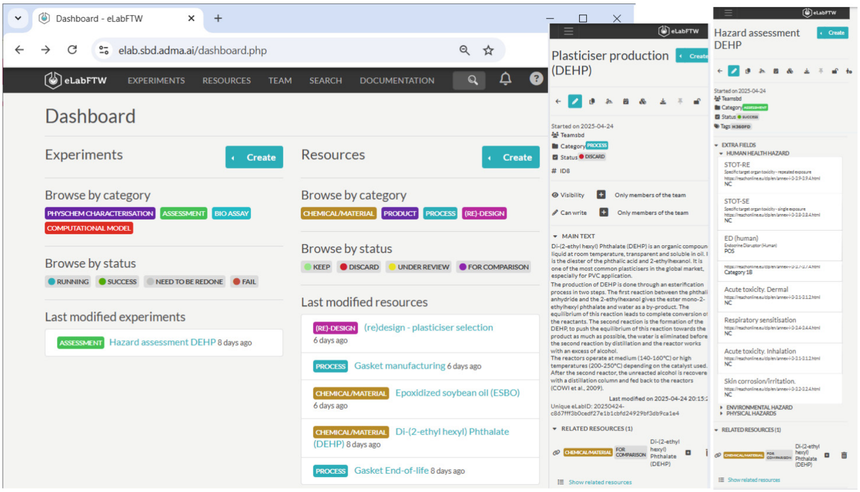
Electronic Laboratory Notebooks (ELN) are digital systems designed to support structured, traceable, and reproducible documentation of laboratory work, increasingly adopted in both academic and industrial settings to enhance data quality and compliance with FAIR principles. Among available ELNs, eLabFTW [2] is a widely used open-source platform that supports experiment tracking, metadata annotation, and integration with external tools and databases via a robust Application Programming Interface (API). Its architecture allows structured entries for materials, processes, and experimental outcomes, with full audit trails, versioning, and user access control. Importantly for SSbD workflows, ELN allows for specifying explicit relationships between items and ensures consistent, machine-readable records. These characteristics make it a suitable backbone for implementing digitally enabled SSbD workflows, where transparent documentation and traceable co-creation are critical.

Our proposed approach is based on a *graph model of the SSbD process and an ELN*. It ensures that every material, test, and decision is clearly documented, linked to related work, and accessible to all team members. It allows each participant to contribute using a consistent format while also enabling *automation and integration with external tools.*

2 Automated SSbD Workflows Supported by ELN

To operationalize Safe-and-Sustainable-by-Design (SSbD) principles in real-world environments, we propose a modular, automation-friendly workflow centered on a configurable eLabFTW instance (Fig. 1). This approach addresses current fragmentation in SSbD implementation by providing structured data capture, traceability, and interoperability with external hazard and sustainability assessment tools. At the core of this solution is a structured representation of materials, chemicals, processes and products within eLabFTW, mapped directly to the stages of the SSbD framework. These representations are enriched with experimental data, metadata, and assessment results.

The SSbD workflow is modeled as a Directed Acyclic Graph (DAG, illustrated in Fig. 2), where each node represents a resource (material, process, product) and each directed edge points to an upstream dependency or input relation. Iteration - an essential aspect of SSbD - is encoded through decision nodes, representing the re-design step. The decisions are reflected by setting the upstream resource status to “keep” or “discard”, and a timestamp of the decision, providing a clear record of evaluations over time. A new iteration can be recorded either by adding an upstream resource to an existing decision node (i.e. new alternative) or by introducing a new decision node (e.g. a new re-design step). Each resource is assigned a persistent entry in the eLabFTW, with typed metadata and links to upstream dependencies via the “linked resources” field. Decision nodes are modeled as dedicated resources of type “(re)-design”, documenting the rationale, timestamp, and outcome of material or process selection steps. Experimental data (hazard assessments, performance tests, material characterization) are recorded as experiments (a persistent entry in the eLabFTW) and are linked to the corresponding resources. Experiment templates are defined for different types of assessments and lab experiments.



Dashboard

Experiments

Browse by category
PHYSCHEM CHARACTERISATION
ASSESSMENT
BIO ASSAY
COMPUTATIONAL MODEL

Browse by status
RUNNING
SUCCESS
NEED TO BE REDONE
FAIL

Last modified experiments
ASSESSMENT Hazard assessment DEHP 8 days ago

Resources

Browse by category
CHEMICAL/MATERIAL
PRODUCT
PROCESS
(RE)-DESIGN

Browse by status
KEEP
DISCARD
UNDER REVIEW
FOR COMPARISON

Last modified resources
(RE)-DESIGN (re)design - plasticiser selection 6 days ago
PROCESS Gasket manufacturing 6 days ago
CHEMICAL/MATERIAL Epoxidized soybean oil (ESBO) 6 days ago
CHEMICAL/MATERIAL Di-(2-ethyl hexyl) Phthalate (DEHP) 8 days ago
PROCESS Gasket End-of-life 8 days ago

Plasticiser production (DEHP)

Started on 2025-04-24
Teamsbd
Category PROCESS
Status DISCARD
ID8

Visibility Only members of the team
Can write Only members of the team

MAIN TEXT

Di-(2-ethyl hexyl) Phthalate (DEHP) is an organic compoun
liquid at room temperature, transparent and soluble in oil. I
is the diester of the phthalic acid and 2-ethylhexanol. It is
one of the most common plasticisers in the global market,
especially for PVC application.

The production of DEHP is done through an esterification
process in two steps. The first reaction between the phthali
anhydride and the 2-ethylhexanol gives the ester mono-2-
ethylhexyl phthalate and water as a by-product. The
equilibrium of this reaction leads to complete conversion o
the reactants. The second reaction is the formation of the
DEHP, to push the equilibrium of this reaction towards the
product as much as possible, the water is eliminated before
the second reaction by distillation and the reactor works
with an excess of alcohol.
The reactors operate at medium (140-160°C) or high
temperatures (200-250°C) depending on the catalyst used.
After the second reactor, the unreacted alcohol is recovere
with a distillation column and fed back to the reactors
(COWI et al., 2009).

Last modified on 2025-04-24 20:15:
Unique eLabID: 20250424-c867fff3b0cedf27e1b1cbfd24929bf3db9ca1e4

RELATED RESOURCES (1)
CHEMICAL/MATERIAL FOR COMPARISON Di-(2-ethyl hexyl) Phthalate (DEHP)
Show related resources

Hazard assessment DEHP

Started on 2025-04-24
Teamsbd
Category ASSESSMENT
Status SUCCESS
Tags H360FD

EXTRA FIELDS
HUMAN HEALTH HAZARD

STOT-RE
Specific target organ toxicity - repeated exposure
https://reachonline.eu/clp/en/annex-i-3-3.9-3.9.4.html
NC

STOT-SE
Specific target organ toxicity - single exposure
https://reachonline.eu/clp/en/annex-i-3-3.8-3.8.4.html
NC

ED (human)
Endocrine Disruptor (Human)
POS

https://reachonline.eu/clp/en/annex-i-3-3.7-3.7.4.html
Category 1B

Acute toxicity. Dermal
https://reachonline.eu/clp/en/annex-i-3-3.1-3.1.2.html
NC

Respiratory sensitisation
https://reachonline.eu/clp/en/annex-i-3-3.4-3.4.4.html
NC

Acute toxicity. Inhalation
https://reachonline.eu/clp/en/annex-i-3-3.1-3.1.2.html
NC

Skin corrosion/irritation.
https://reachonline.eu/clp/en/annex-i-3-3.2-3.2.4.html
NC

ENVIRONMENTAL HAZARD
PHYSICAL HAZARDS

RELATED RESOURCES (1)
CHEMICAL/MATERIAL FOR COMPARISON Di-(2-ethyl hexyl) Phthalate (DEHP)
Show related resources

Fig. 1. Dashboard view of the eLabFTW instance used for implementing SSbD workflows. Resources and experiments are categorized by type and by status. Each resource has a dedicated page with metadata, linked experiments and resources.

This approach allows the entire SSbD lifecycle (design, synthesis, testing, and selection to end-of-life considerations) to be expressed as a connected graph, ensures traceability while preserving the ability to backtrack and improve designs based on new data.

Assessment information can be added either manually or automatically. Figure 1 (right) shows a screenshot of the Hazard assessment template, listing required SSbD fields.

Automation is supported through the eLabFTW API, enabling workflows that launch external tools such as computational models (e.g., QSAR models for property prediction, or external models for predicting performance) or data services that query toxicological databases. This flexibility allows integration of both expert input and algorithmic evaluation to support decision-making in the SSbD process. A Python-based workflow has been implemented to traverse the SSbD resource graph via the eLabFTW API. This automated pipeline extracts relevant metadata, hazard and performance data, and decision outcomes to generate comprehensive SSbD documentation, including tabulated hazard summaries and visualizations (Fig. 2).

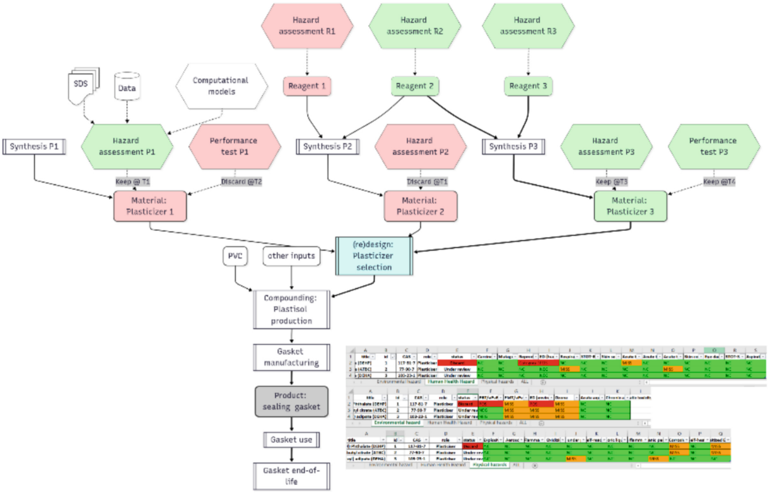


Fig. 2. Directed Acyclic Graph (DAG) representing the SSbD workflow for plasticizer substitution in gasket production [3]. Rectangle nodes represent materials, processes, and decision points. Hexagon nodes represent evaluations (hazard, performance, sustainability, etc.). Directed edges indicate upstream dependencies. Each node has a dedicated page in eLabFTW, containing structured metadata, upstream links, and associated experimental evidence. Bold arrows trace the selected SSbD path based on hazard and performance criteria.

3 Implementation and Case Studies

3.1 Case Study: Plasticizer Substitution

We applied this approach to a representative case study from the European Commission's SSbD framework: the selection of safer plasticizers for PVC-based gasket production, as described in JRC131878 report [3]. Using eLabFTW, each material (e.g., plasticizer candidates, PVC), process (e.g., synthesis, compounding, gasket manufacturing) and the final product are modeled as resources. Hazard assessments and performance tests are recorded as experiments and linked to materials, while decision points (e.g., the plasticizer selection) are modeled as a resource of type "(re)-design" (Fig. 2). The resulting DAG captures the full SSbD reasoning path, from reagents through synthesis, performance and hazard evaluation, material selection, manufacturing, and eventual product fate. Decision nodes document the rationale for keeping or discarding candidates based on screening outcomes. For example, a safe "Plasticizer 1" is discarded after poor performance testing; "Plasticizer 2" is discarded due to unfavorable hazard assessment results. The selected "Plasticizer 3" passed both assessments and is incorporated into the final gasket product. Decision timestamps (T1, T2, T3) record the outcomes at each stage, documenting when and why a resource is retained or excluded. The SSbD hazard assessment tables (Fig. 2) are generated automatically with a Python script. The ELN with this case study is publicly available at https://elab.sbd.adma.ai/.

3.2 Case Study: ZEROF Textile

In a second case study, we present the directed acyclic graph representing the ZEROF SSbD workflow [4] for the development and optimization of an ORMOCER-based coating applied to different fabrics (Fig. 3). The DAG encodes the full SSbD lifecycle, from precursor selection and synthesis to material characterization, performance testing, and final product application. Multiple synthesis routes are explored (O1 and O3 included only for clarity), each involving distinct combinations of reagents. Followed by performance evaluation based on contact angle measurements. Decision points mark materials as "keep" or "discard" with associated timestamps, enabling iterative refinement. The coating is then applied to selected fabrics, optionally incorporating additives, each evaluated for hazard and performance. Final product formation leads to downstream life cycle stages, including installation, use, and disposal. Hazard, sustainability, and economic assessments are attached to the nodes, with data sources including safety data sheets, computational models, and curated databases. The graph structure preserves traceability and supports upstream and downstream traversal. The ELN instance with this case study is available within the ZEROF project space at https://enanomapper.adma.ai/ and is accessible by project partners only.

Figure 3 illustrates the complexity of exploring the design space for new material development – there are multiple design decisions (blue boxes), majority of them related to the performance of the new chemical or material, however, the SSbD framework mandates safety assessment for every chemical (raw materials, reagent, solvents additive, etc.) involved in the different stages of the new material development. Material synthesis is followed by analytical characterisation (e.g. spectroscopy) to confirm the reaction completion and the expected material structure, and performance tests to assess water and oil repellence. The ELN is a native environment to store such experimental data, and the graph structure ensures linking this information to design decisions. Similarly, computational models are represented as eLabFTW experiments and linked to e.g. hazard or performance assessments.

Creating a chemical/material resource in eLabFTW requires specifying the substance identity. Partners can add materials through the web interface and link them to a specific SSbD stage. A Python workflow was developed to integrate and retrieve data from multiple relevant databases and launch property predictions using existing QSAR models (VEGA, ToxTree, custom models), and these could be automatically written back to the ELN. The approach improves traceability of the decisions through explicit links and ensures data integration and automation.

SSbD reports, as hazard assessments (tables) and graphs (as in Fig. 2 and Fig. 3), are generated using the eLabFTW API and an open-source Python workflow. Future developments include an online user interface for report generation, tools for handling conflicting outputs of predictive models and AI assistants to help compile the hazard assessments based on unstructured data.

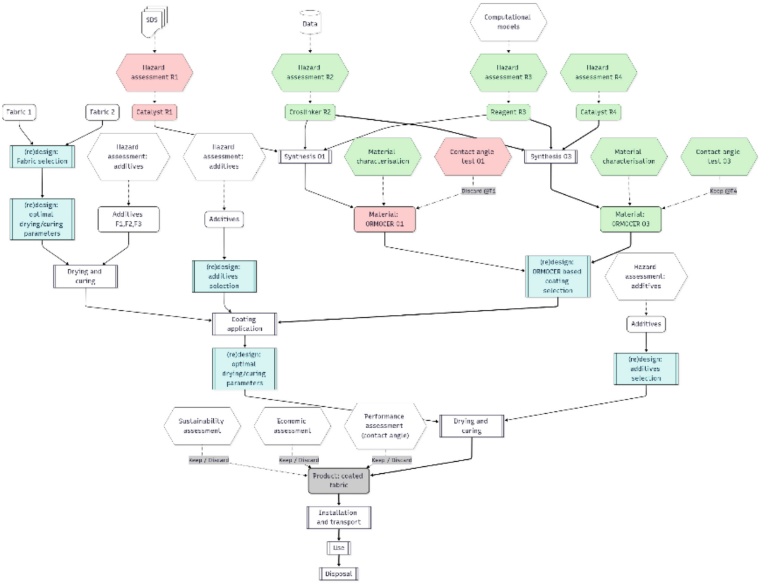


Fig. 3. Directed Acyclic Graph representing the SSbD workflow for development and selection of ORMOCER-based coatings for textiles. Rectangle nodes represent materials, synthesis steps, products and decisions (blue), with directed edges capturing dependencies. Hexagon nodes represent lab experiments or assessments. Each graph node corresponds to a dedicated page in eLabFTW with its own identifier, content, metadata, linked experiments, timestamp and decision rationale.

4 Discussion and Conclusions

SSbD represents a *reuse* scenario in the FAIR data paradigm, where data and workflows originally generated for regulatory safety assessment or life cycle analysis are repurposed to support early-stage innovation. Unlike traditional safety assessments, which are typically conducted by certified toxicologists at later stages of product development and in a data-rich environment, SSbD requires non-specialists, such as materials scientists or engineers, to engage with safety and sustainability metrics from the early stages of the innovation. To address this challenge, we propose an approach that embeds experimental records, metadata, and decision logic within an Electronic Laboratory Notebook (ELN), and structures their interdependencies as a Directed Acyclic Graph (DAG). While an ELN facilitates data and metadata organisation, it does not mandate specific data formats for experimental results; therefore, we aim to build on a decade of experience in the co-creation of domain-specific data entry templates and user-guided tools as the Template Wizard [5].

The approach is applicable to any FAIR-compliant ELN that supports resource linking and programmatic access. A key enabler is the capacity of ELNs to serve as more than static documentation tools: but as dynamic hubs for automation, while remaining complementary to the dedicated decision support systems. Through well-defined APIs, both internal scripts and external services can read from and write to the ELN in real time – enabling integration with laboratory instruments, data analysis pipelines, AI-based predictive models, sustainability calculators, and external knowledge bases, as well as visualization of alternative material choices and their impact pathways. We anticipate that ELN will evolve into a digital workspace within an ecosystem of interoperable tools, coordinating structured data flows across the entire innovation lifecycle, and thus addressing the co-creation gap in SSbD research. The architecture has the potential to make SSbD more accessible to interdisciplinary teams and better aligned with evolving regulatory, sustainability, and innovation frameworks. Future applications and new developments of the approach will be available at https://sbd.adma.ai.

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