Methodological challenges and ways forward for SSbD

ECETOC's Annual Technical Meeting

23 May 2024

Peter Fantke
Technical University of Denmark

Proposed SSbD framework: Objectives

- **Drive innovation toward SSbD new** chemicals/materials
- **Provide guidance** on SSbD design criteria development
- **Minimise/eliminate life cycle impacts** on humans, climate & environment
  - Phase out **existing most harmful substances**
  - Substitute **existing substances of concern**, and minimise their production/use
- **Enable comparative assessments of new/existing** chemicals/materials for a given function or application context

by design

- **Molecular design** based on chemical structure
- **Process design** for safer production processes
- **Product design** for supporting selection of solutions meeting functional product demands

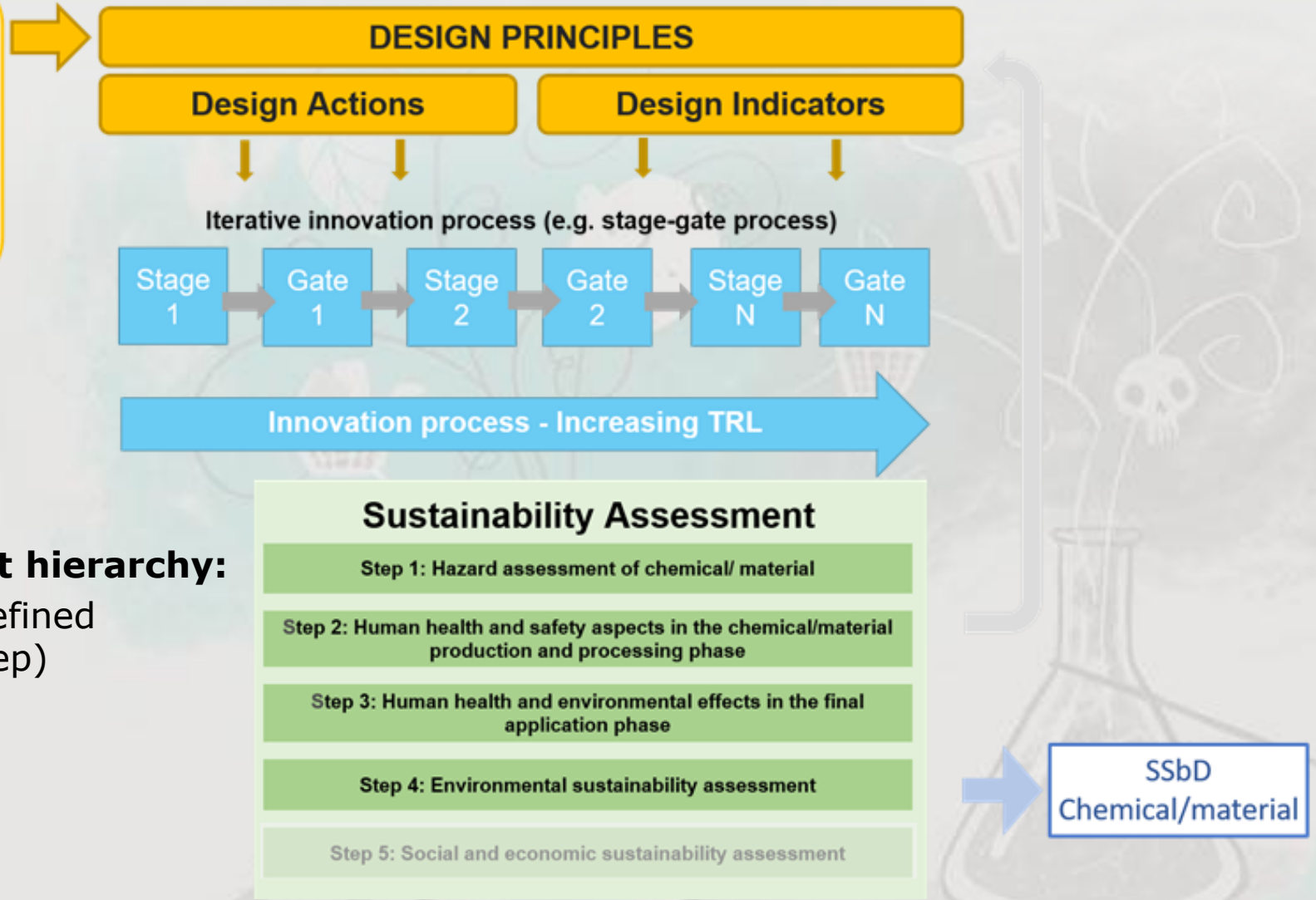
Design principles

1 - Material efficiency
2 - Minimise use of hazardous chemicals/materials
3 - Design for energy efficiency
4 - Use renewable ressources
5 - Prevent & avoid hazardous emissions
6 - Reduce exposure to hazardous substances
7 - Design for end-of-life
8 - Consider whole life cycle

Application of proposed SSbD framework

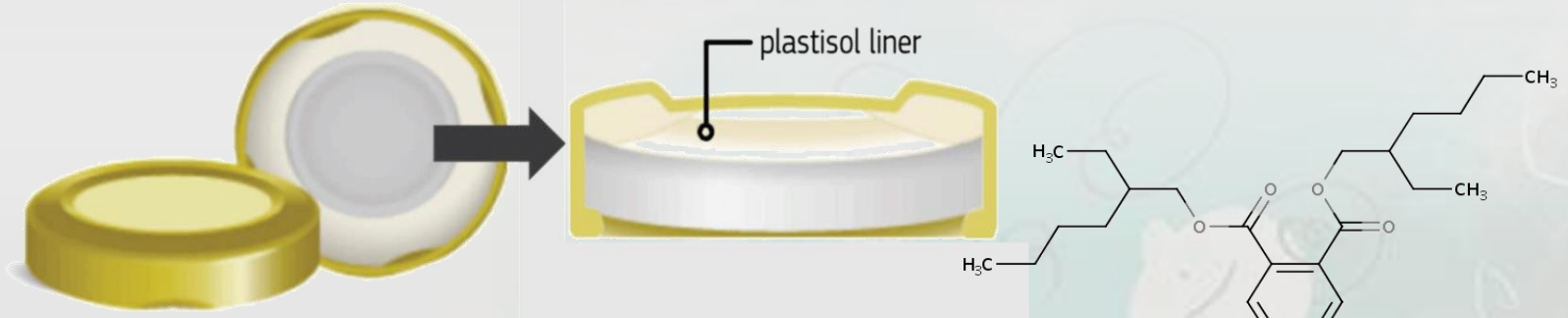
Strategies and principles can be followed such as:

- Green chemistry
- Green engineering
- Sustainable Chemistry
- Safe by design
- ...

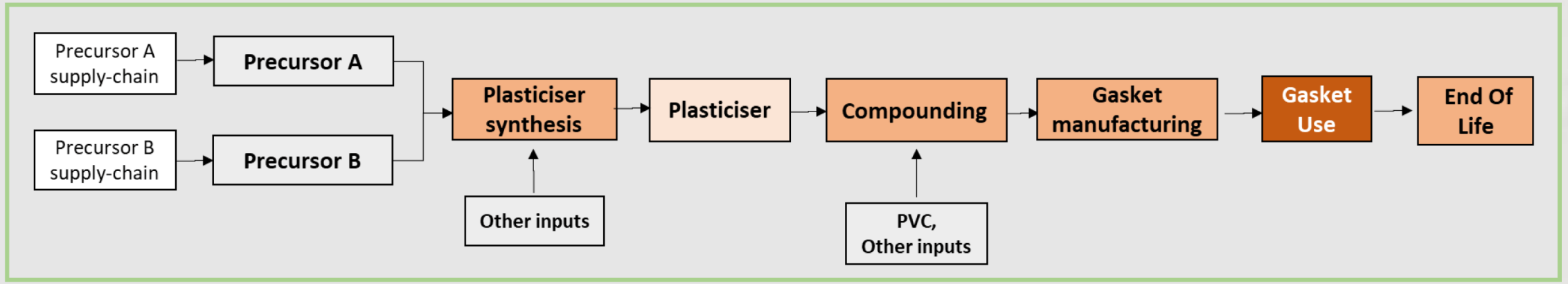


SSbD assessment hierarchy:
(based on set of defined criteria for each step)

Example JRC case study: Plasicisers in FCM



Step 1: Plasticizer | Step 2: Processing steps where the plasticizer is present | Step 3: Final application phase | Steps 4: Entire life cycle



Associations contacted:

CEFIC/ European Plasticisers

PlasticsEurope/ECVM

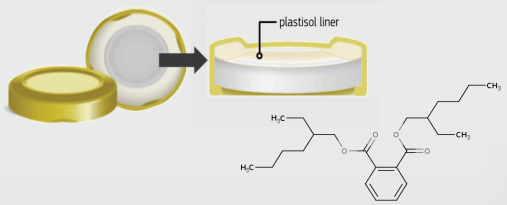
European Council of the Paint, Printing Ink and Artists' Colors Industry

European Plastic Converters

Metal Packaging Europe

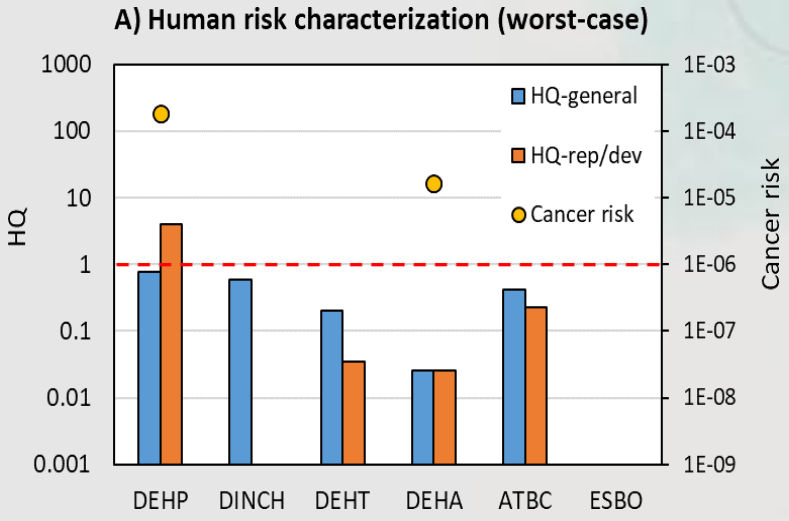
FoodDrinkEurope

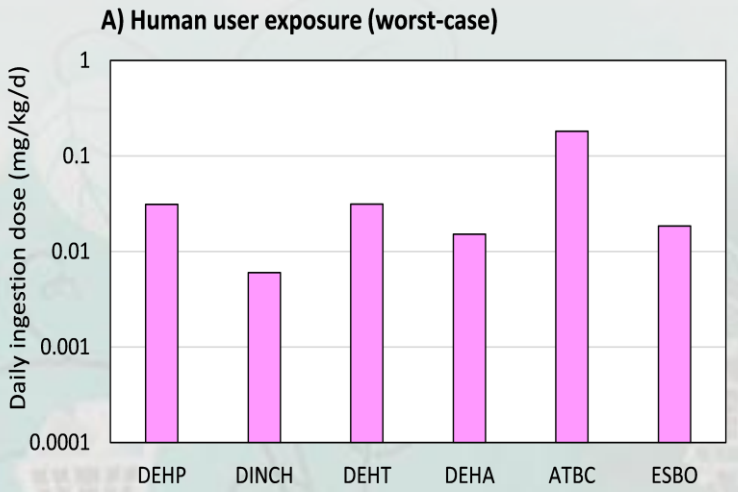
Example JRC case study: Plasicisers in FCM results

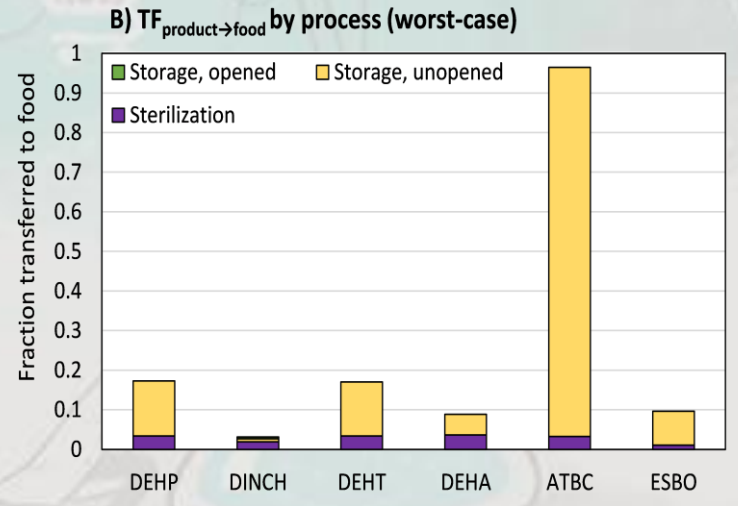


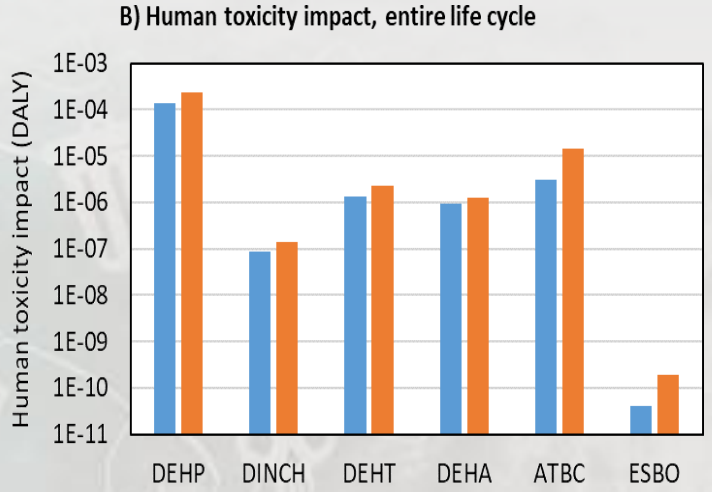
USEtox tool (www.usetox.org)

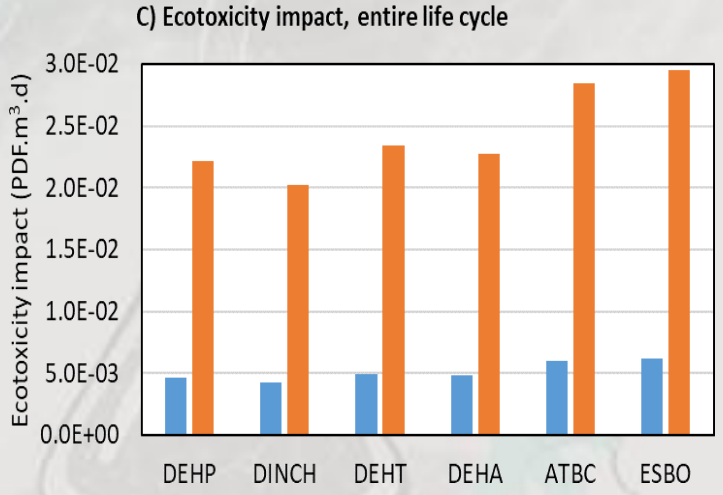
- Full mass balance
- Scientific consensus-bases
- Aligned metrics for SSbD steps











Challenges – Hazard and exposure domain

Chemical and material data gaps

— lack of chemical property and hazard data

— robust use of new approach methods (NAMs)

— application, use patterns

— availability of design-stage data

Missing assessment methodology

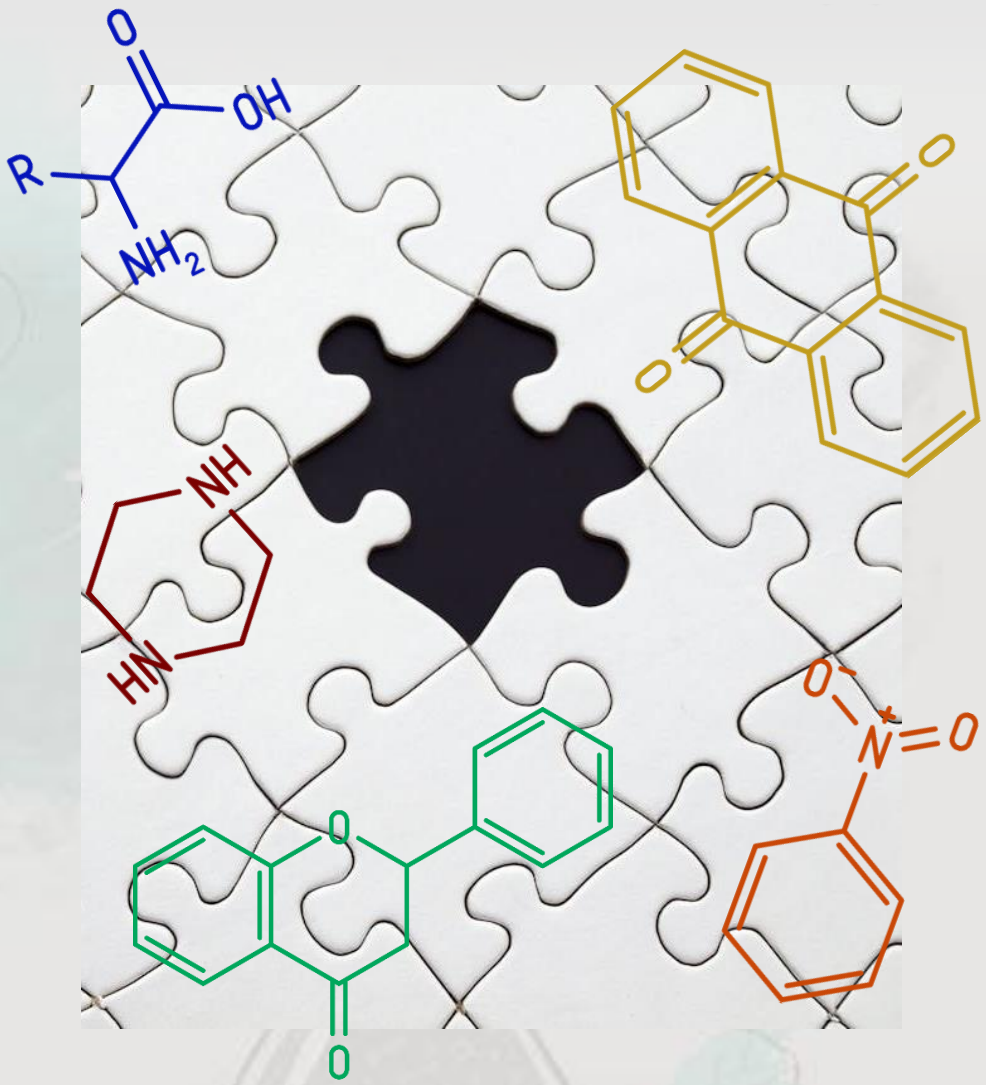
— Approaches for mixtures, formulations

— Novel substances, e.g. nanomaterials, bio-based chemicals

Function-based assessment

— function at chemical/material/technology levels

— scaling across functional levels



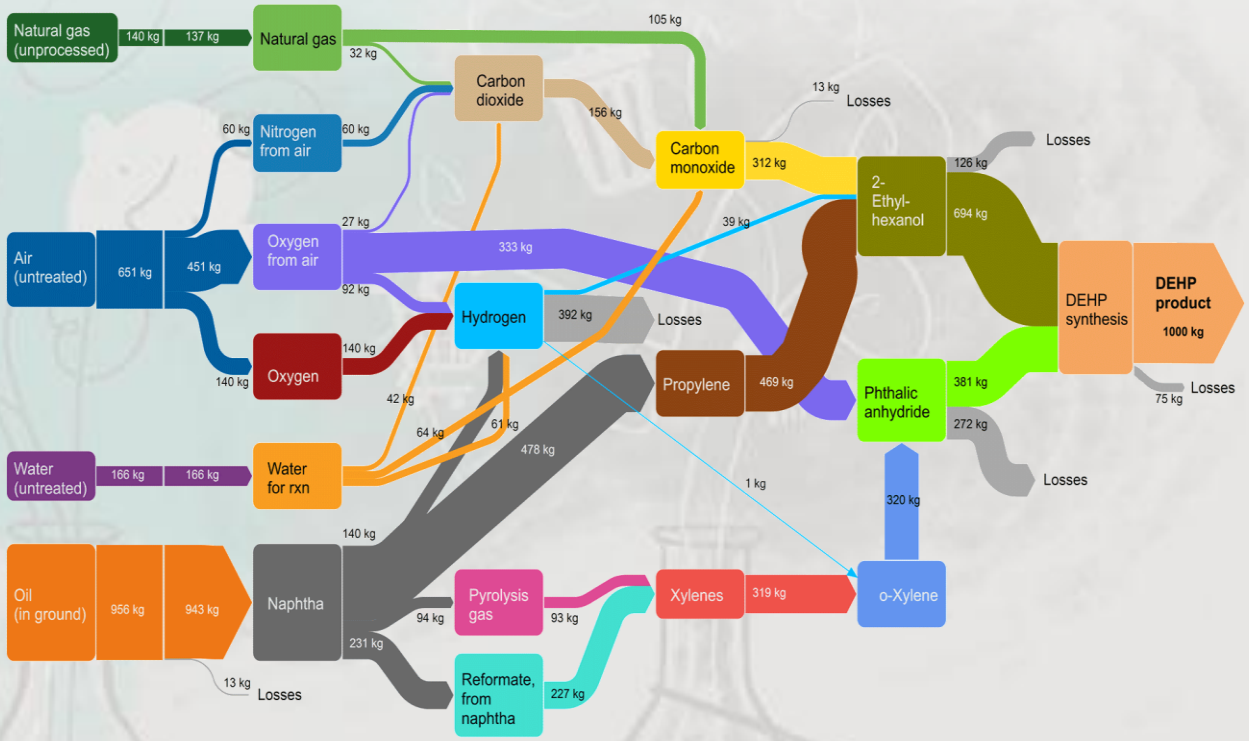
Challenges – Sustainability domain

Chemical/material inventory analysis

– Boundary conditions & assumptions
– Data transparency
– Prospective inventory analysis
– Upscaling methods

Impact assessment

– Streamline impact category selection
– Combing/aggregating impacts
– Environmental damage modelling
– Inclusion of social aspects



Challenges – Decision domain: "good enough" solutions

Definition of safety targets

– Identifying chemical groups of concern and "safe" chemical-use combinations

– Defining "safe" exposure levels / acceptable risks

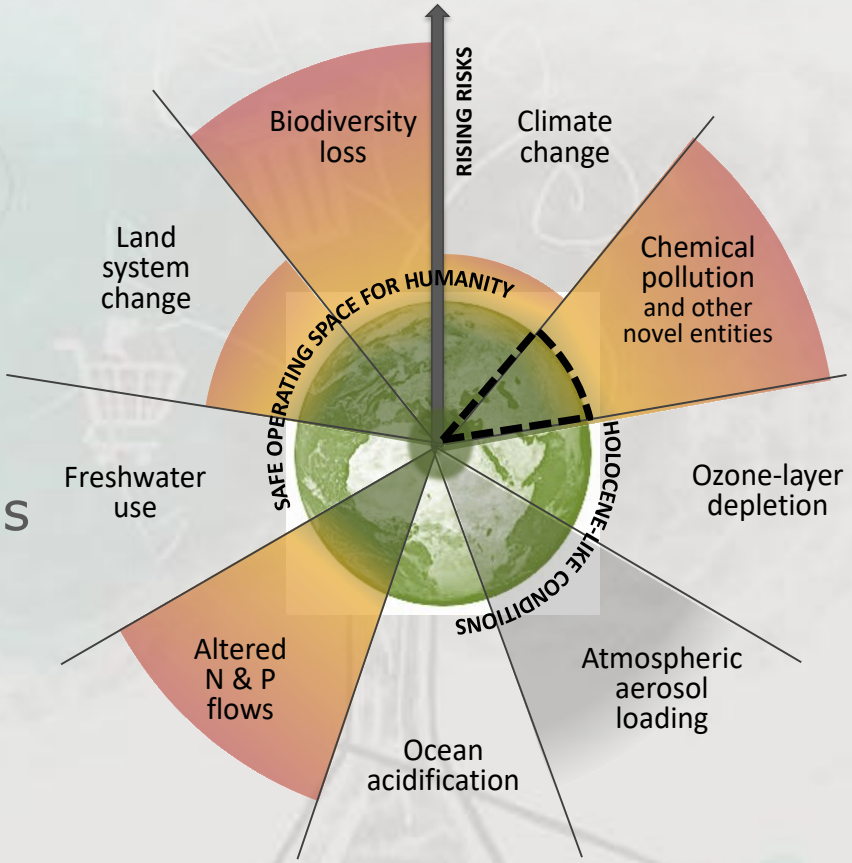
Definition of biophysical sustainability targets

– Selecting relevant target & spatiotemporal domains

– Defining missing targets (chemicals, plastics)

– Linking impacts to targets

– Aggregate biophysical damage



Ways forward – Digitalization & simplification

Develop reliable *in silico* based data

– Inventory & impact assessment

– Expand chemical coverage

Align criteria & metrics

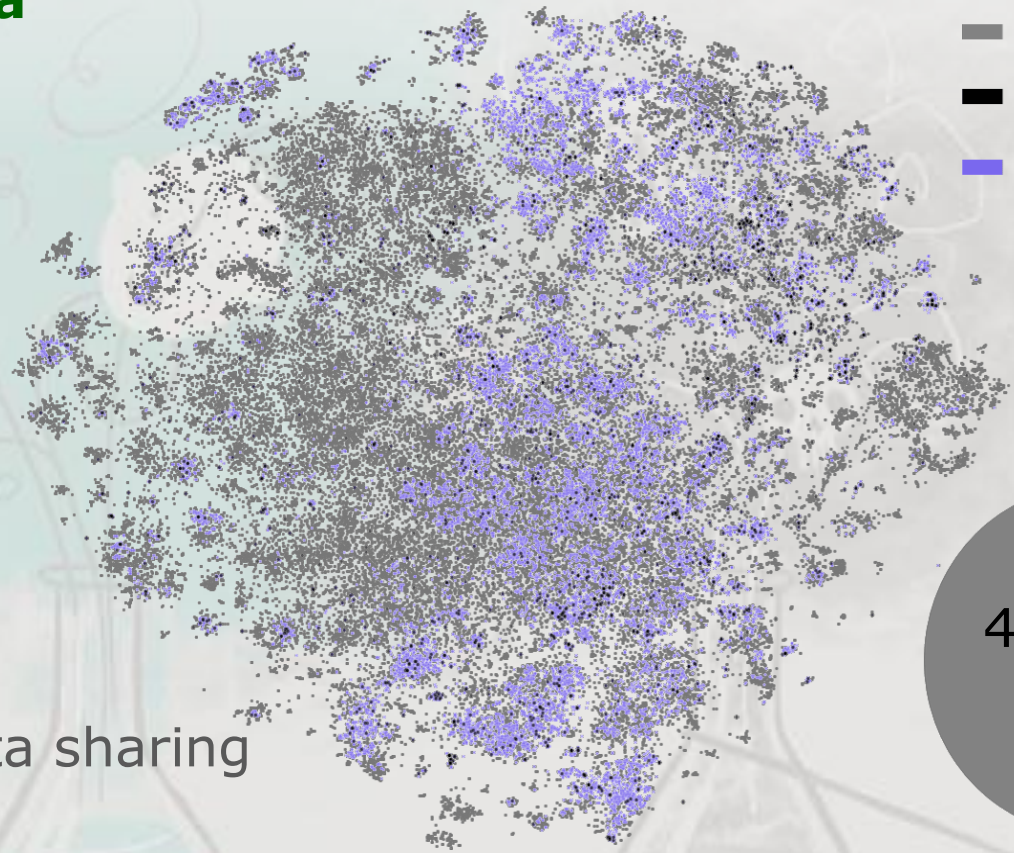
– Across scopes (process vs. use)
& perspectives (emitter vs. receptor)

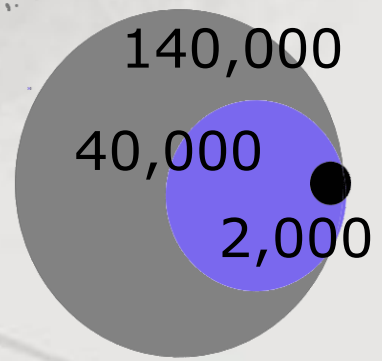
– Function-based approach

Knowledge sharing platforms

– Cross-disciplinary knowledge and data sharing

– Complimentary assessment steps





Ways forward – Collaboration & consensus building

Establish scientific targets

— Absolute sustainability framework

— Mission-driven innovation

Develop flexible consensus tools

— Adapt to various decision contexts

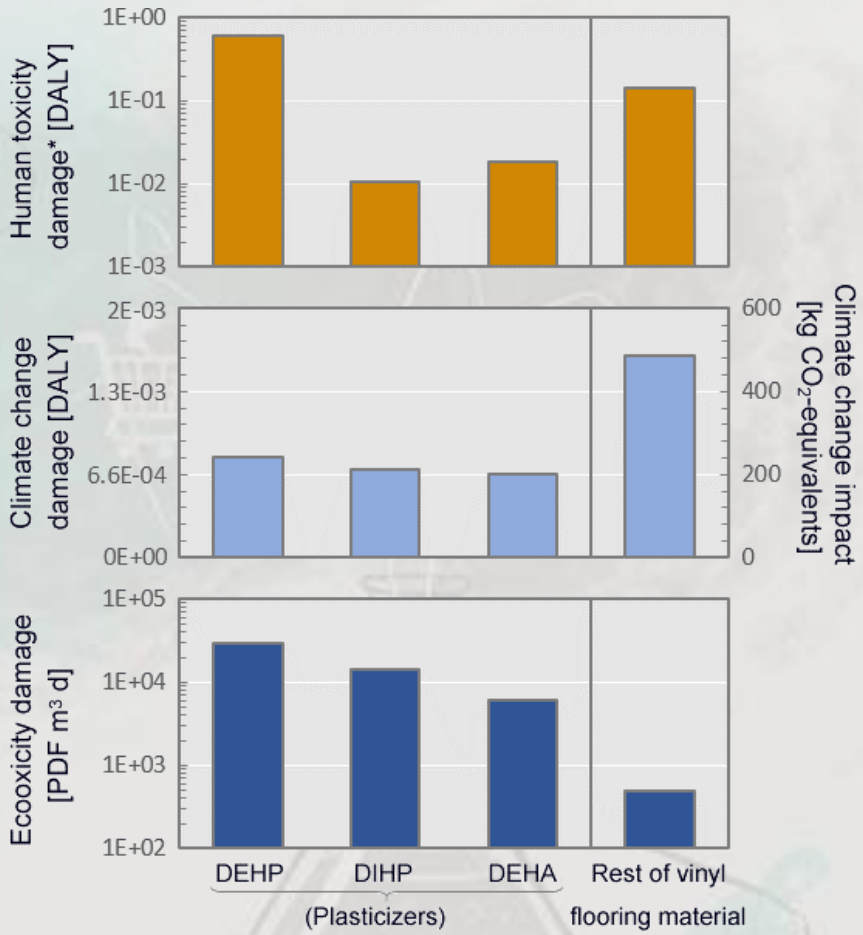
— Scientific consensus approaches

Adapt methods for internal workflows

— Modular assessment framework

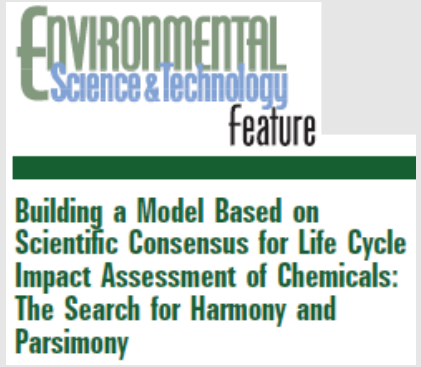
— Open interfaces for companies

— Consider data confidentiality

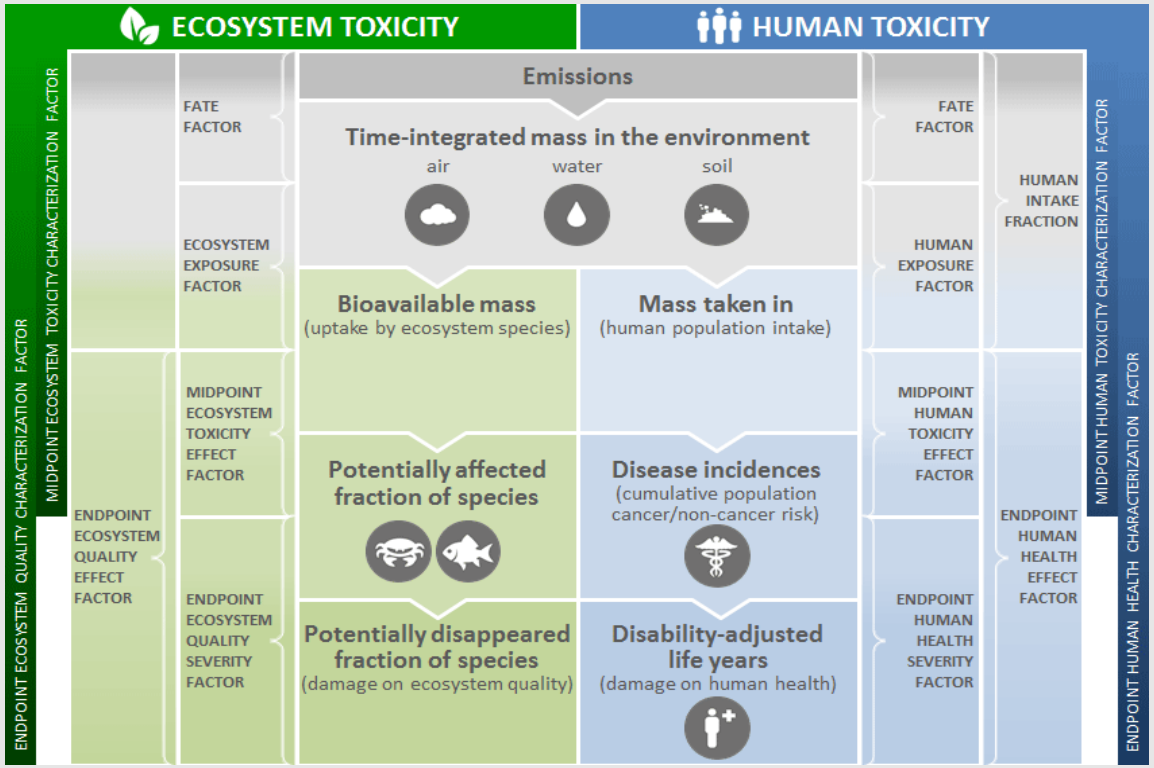


Ways forward – Consensus building in SSbD

- Global UNEP/SETAC **scientific consensus** model USEtox
- Defined criteria for consensus:
  - Based on mature science
  - Outputs within outputs of other models
  - Only incl. most influential aspects
  - Endorsed by all involved scientists
  - Transparent and well-documented



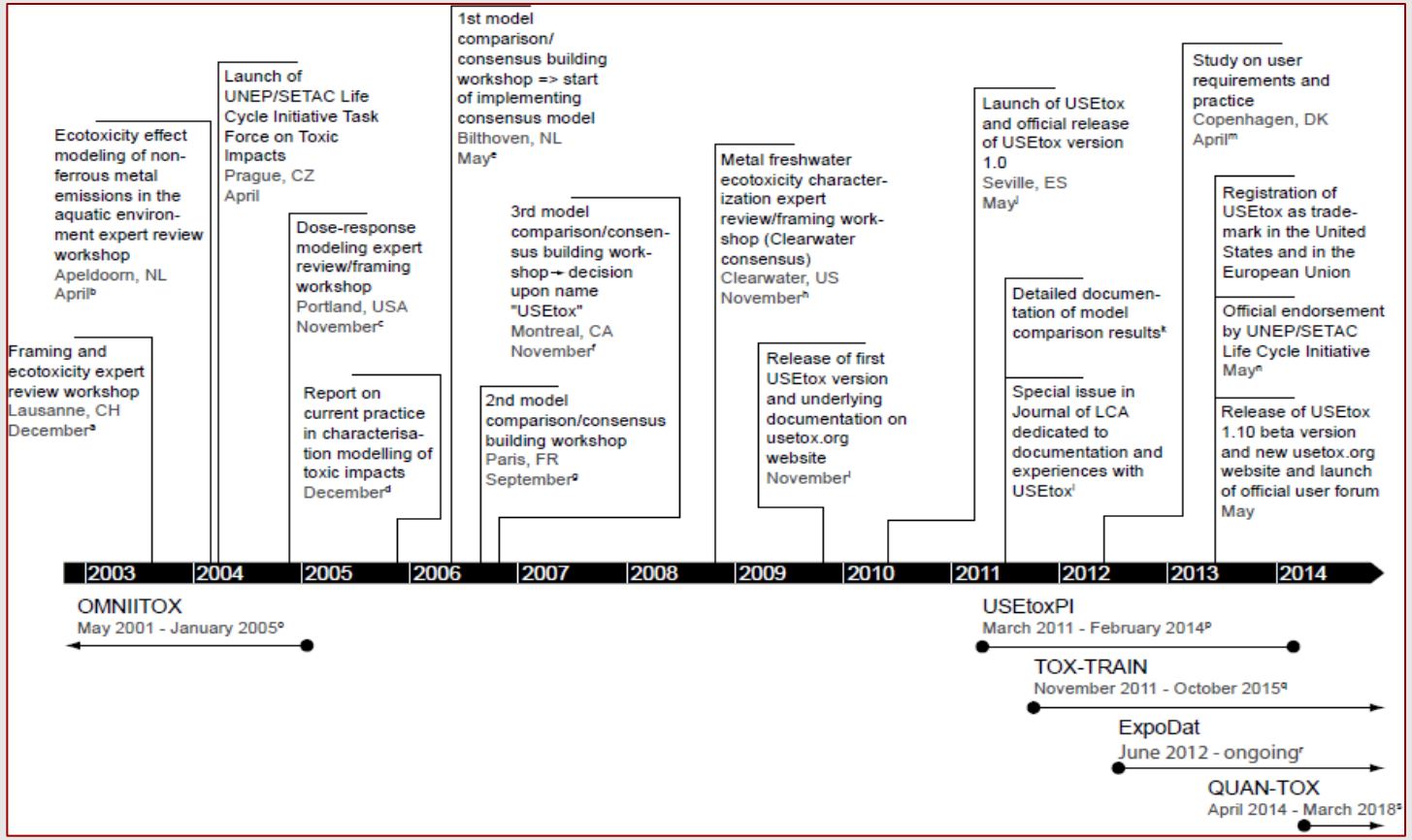
http://doi.org/10.1021/es703145t



http://usetox.org/documentation

Ways forward – Consensus building in SSbD

- Various intl. consensus-building workshops
- Synergistic projects of involved scientists
- No 'best tool' chosen, but consensual model developed, building on components across existing tools
- Ongoing scientific and consensus-building process



http://doi.org/10.1007/s11367-014-0829-8

Ways forward – Consensus building in SSbD

- USEtox continuously further developed (e.g. via UNEP GLAM, UNEP SAICM)
- **Business model**: open & free to use by all, but proper training needed
- Modular assessment framework
- Continuously striving for scientific consensus
- **Metrics** 'fit-for-purpose' for different decision contexts

https://lifecycleinitiative.org/applying-lca/lcia-cf

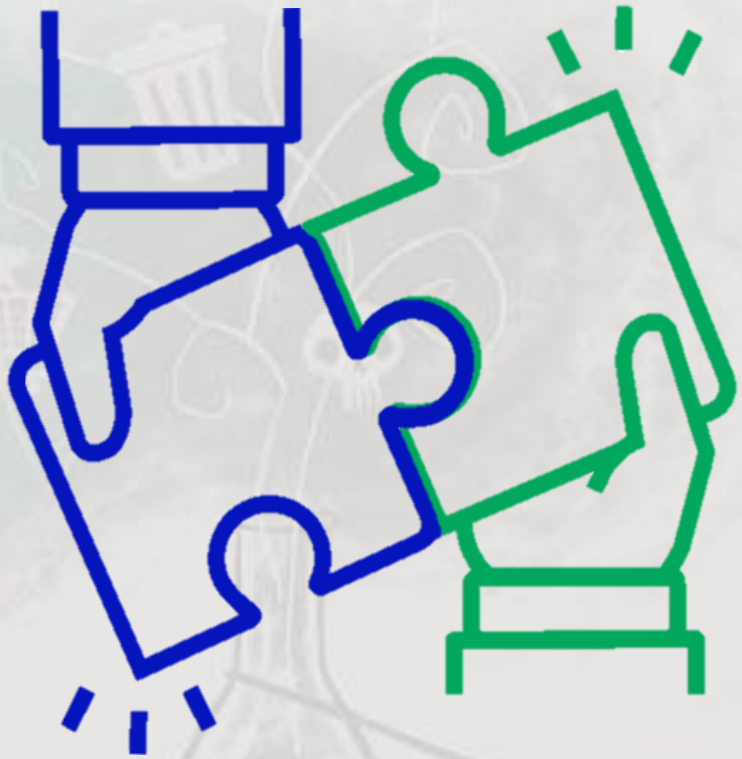
Take-home points

1. SSbD comes with **new research challenges**, but can already build on various existing data, methods and tools

2. SSbD fosters a rigorous **scientific foundation** & developing novel scientific approaches that are fit-for-purpose

3. SSbD needs a strong **consensus-building** effort to become a science-based yet operational and sustainability-driven innovation tool

4. **Collaboration** is key for a stepwise improvement of scientific SSbD methods to go from “better” to “good enough”, i.e. SSbD!



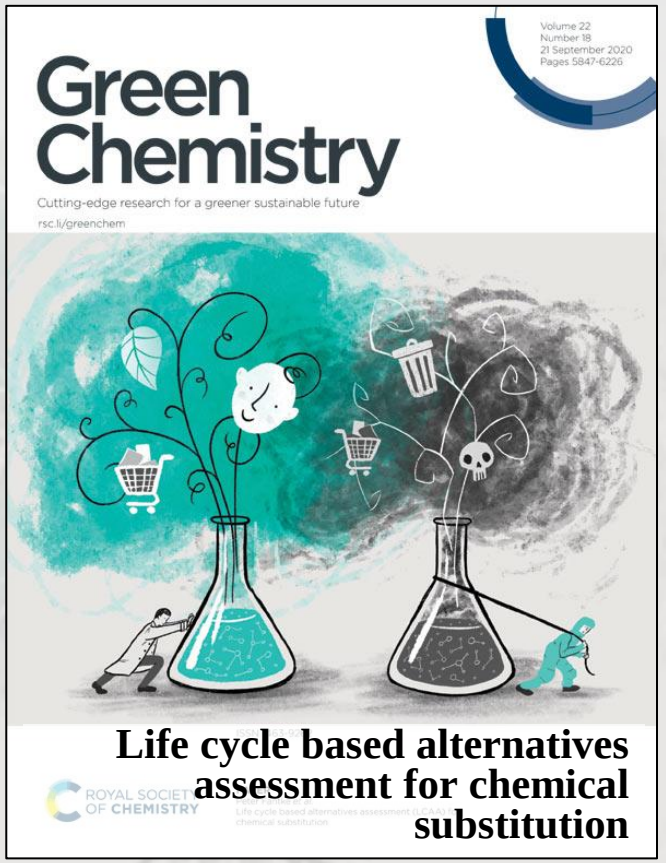
SSbD reports & Example Framework

JRC review

JRC framework

JRC case study

EU recommendations



"SSbD" type framework incl. case study