Materials Science and Technology

PARC case-study BPA and alternative substances: First broad testing of tools for SSbD assessments

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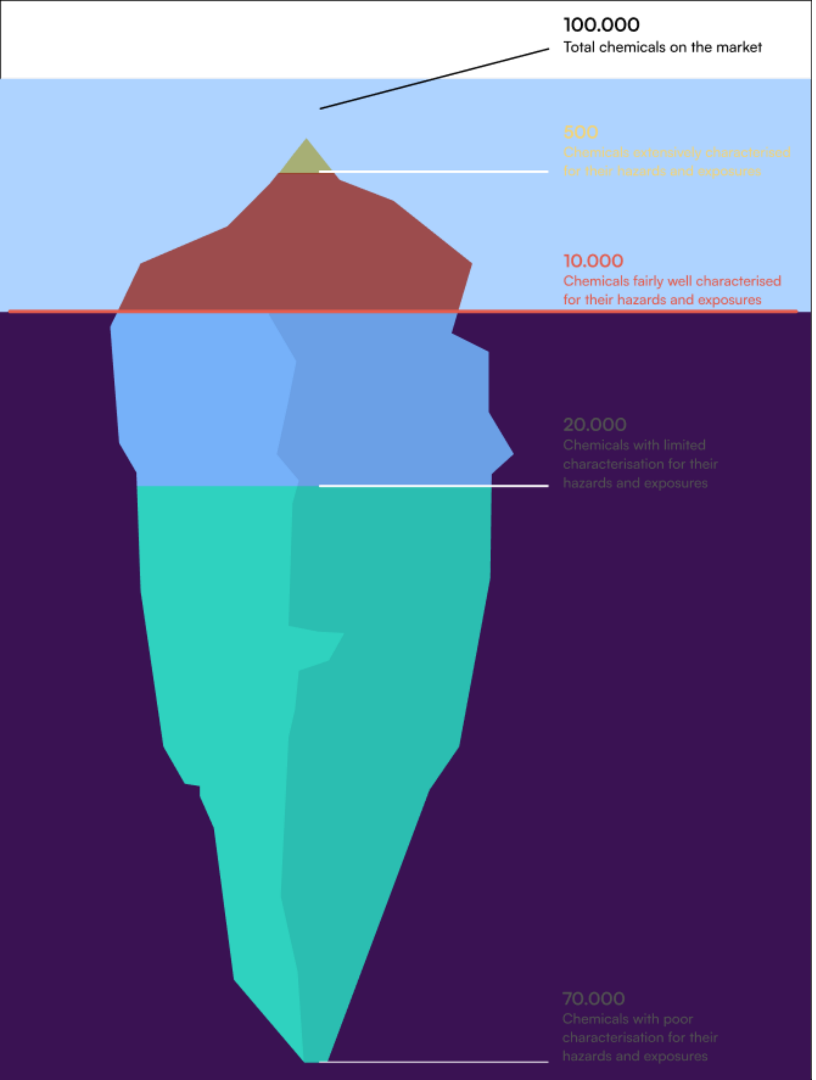
Postdoctoral Researcher at Empa



Safety and sustainability assessments to improve chemical and material management

- (synthetic) chemicals are present everywhere in our daily lives
- Many properties of these chemicals are unknown
- SSbD can be a proactive way to better manage chemicals (and materials) by assessing safety and sustainability
- PARC: developing a toolbox to facilitate the SSbD assessment

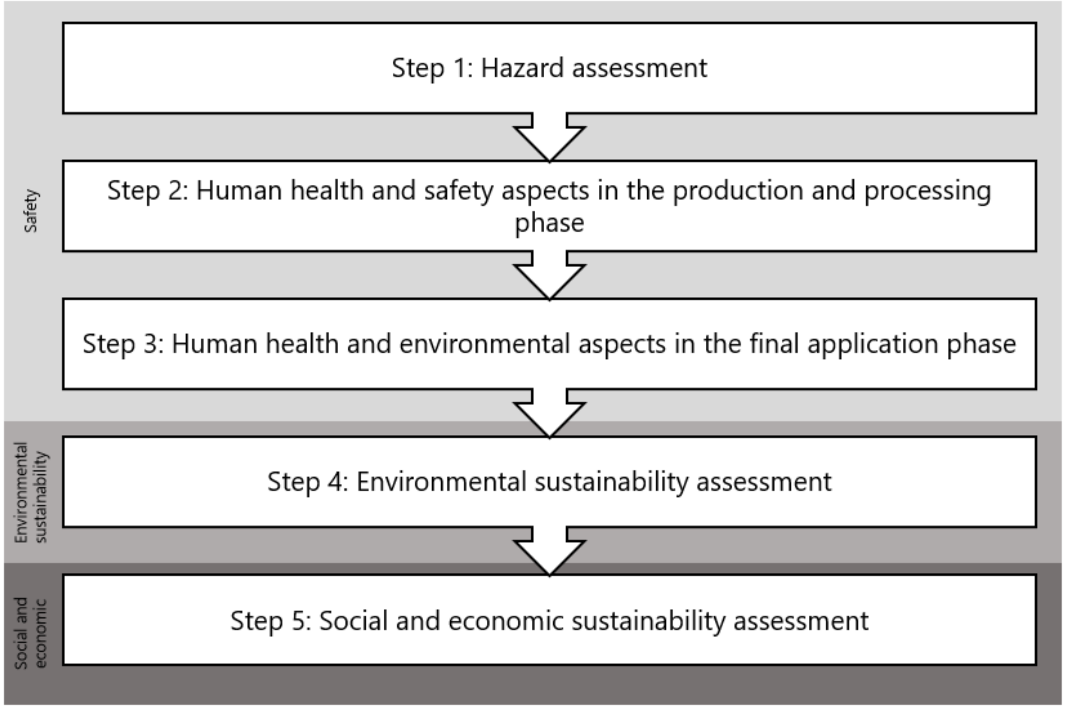
PARC SSbD Toolbox

- Based on the SSbD framework from the J (Caldeira et al.

ent

- these tools

In order to facilitate this, we need to understand how the different tools work

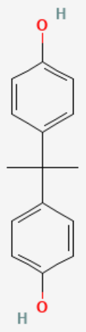


SSbD Assessment Framework (Caldeira et al., 2022)

Aim and selection of the case-study

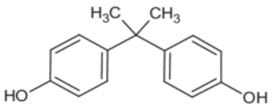
Aim

- Test different chemical structures
- Test the applicability of the tools in relation to different stages of innovation
- Understand the complexity of the tools, and their potential role in SSbD assessments
- Evaluate and understand how the tools predict impacts
- Discuss the prediction accuracy, for example

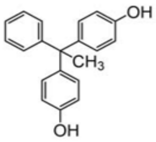


- Bisphenol A (BPA) and two BPA alternatives
- it is being studied extensively within PARC
- Used in the synthesis of commercial plastics, including polycarbonates and epoxy resins
- Incorporated into a wide variety of consumer products

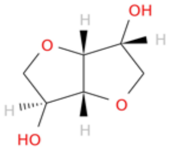
Tested structures and use scenarios



BPA



BPAP

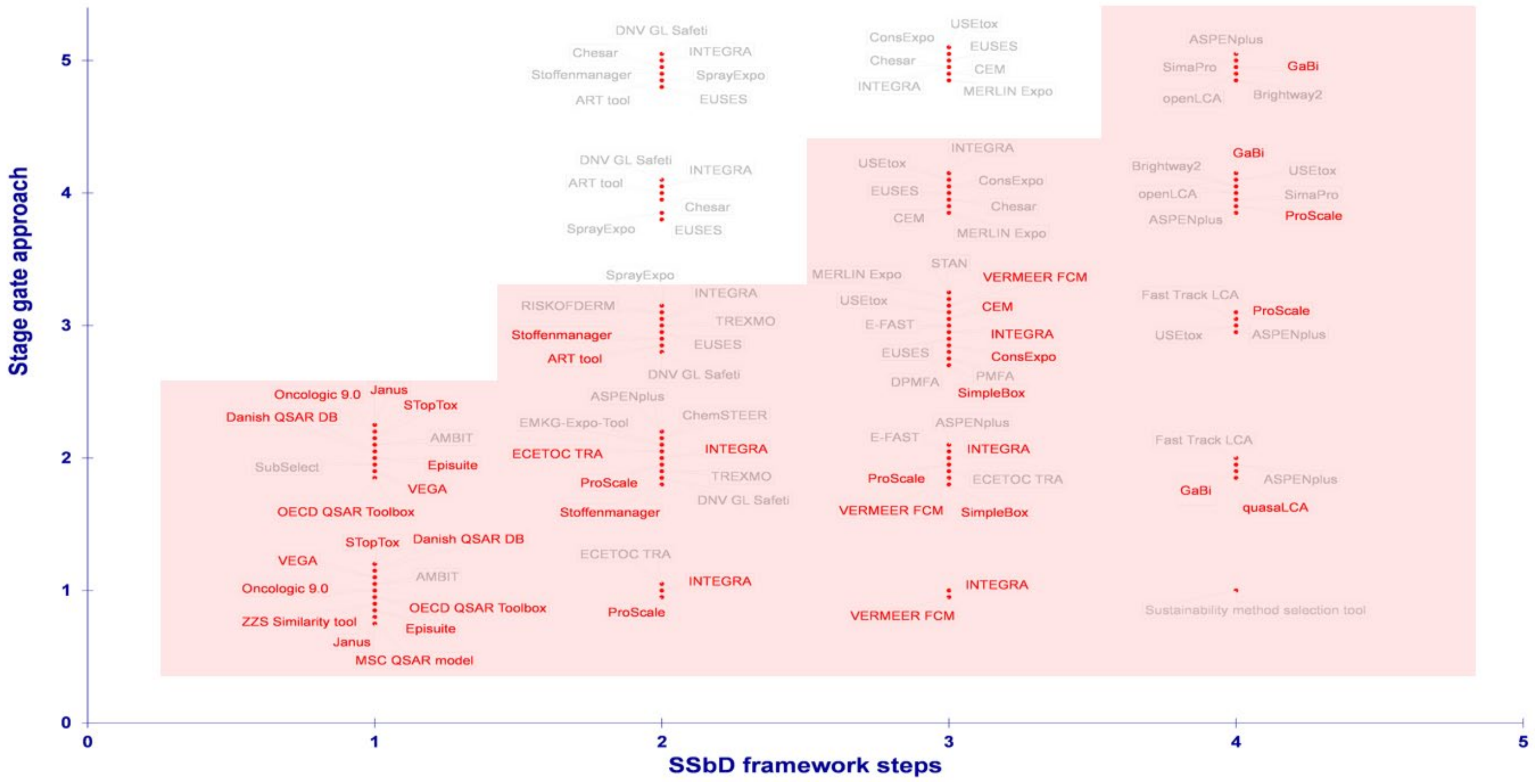


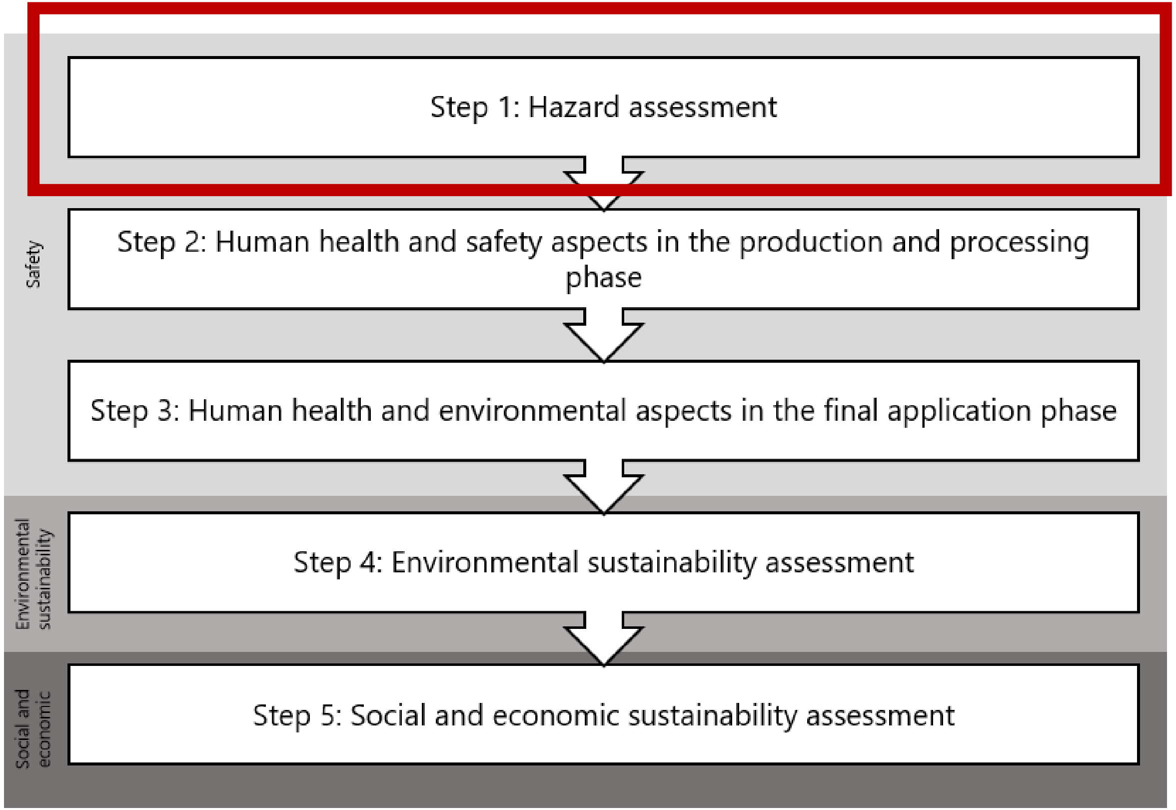
Isosorbide

- Early stage assessment: only the chemical structure and the application of the substance are known.
- Late(r) stage assessment: experimental data available

The tools identified for the toolbox and used in the SSbD assessment

Tools covering different SSbD steps and stage gates




Step 1: Hazard assessment
Step 2: Human health and safety aspects in the production and processing phase
Step 3: Human health and environmental aspects in the final application phase
Step 4: Environmental sustainability assessment
Step 5: Social and economic sustainability assessment
Safety
Environmental sustainability
Social and economic

Step 1: Hazard assessment

- Screening of defined hazard endpoints to identify chemicals that are inherently hazardous.

1. Human health hazards
2. Environmental hazards
3. Physical hazards


European Commission

JRC TECHNICAL REPORT

Safe and Sustainable by Design chemicals and materials

Framework for the definition of criteria and evaluation procedure for chemicals and materials

Caldeira, C. Farcal, R., Garmendia Aguirre, I., Mancini, L., Tosches, D., Amelio, A., Rasmussen, K., Rauscher, H., Riego Sintes, J., Sala, S.

2022

Tested tools

- Danish QSAR DB
- Janus
- EpiSuite v 4.10
- VEGA 1.2.3
- Oncologic 9.0
- OECD QSAR Toolbox
- STopTox

Hazard assessment: scoring approach

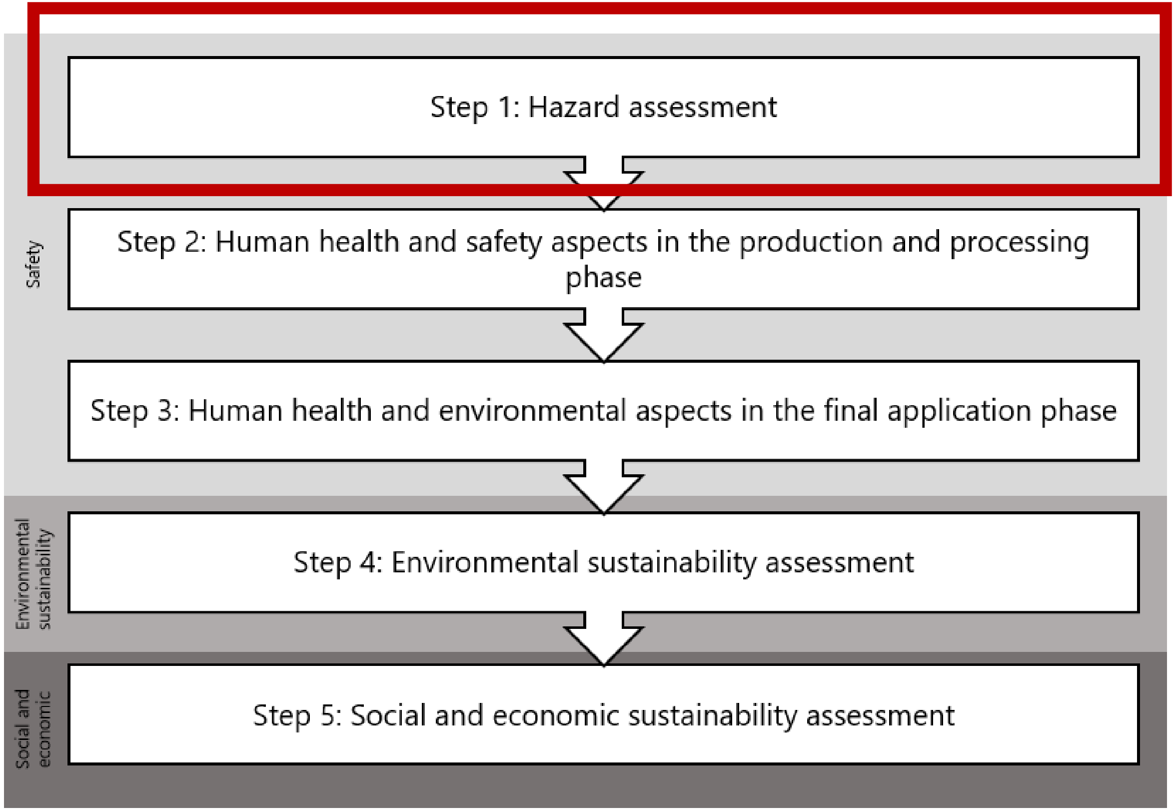
Chemicals	Human health hazards													
	Carcinogenicity	Mutagenicity	Reproductive toxicity	ED (HH)	Respiratory sensitization	STOT-RE	Skin sensitization	Acute toxicity – oral	Acute toxicity – dermal	Acute toxicity – inhalation	Skin corrosion/irritation	Eye damage/irritation	Aspiration hazard	STOT-SE
BPA	NC	NC	Repr. 1B	POS	NC	NC	Skin Sens. 1	NC	NC	NC	NC	Eye Dam. 1	NC	STOT-SE 3
BPAP	NEG	NEG	POS	POS	POS	MISS	NC	NC	NC	NEG	NC	NC	NC	MISS
Isosorbide	NEG	NC	NC	NEG	NEG* POS**	NC	NC	NC	NC	NC	NC	NC	NC	MISS

* Negative prediction within the applicability domain of the model

** Positive prediction within the applicability domain of the model

Step 1: conclusion of the tools

- Not all required endpoints could be covered by using models only
- Guidance needs to be developed on how to integrate different results with each other
  - Conflicting results
  - Experimental and modelled data
  - Data gaps
- Better assessment needed of the uncertainty of both modelled and experimental data



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Step 2: exposure and risk during processing and production

- Information requirements:
  - General physicochemical properties of the substance (molecular weight, vapor pressure), toxicological information:
    - Early innovation: QSAR results step 1 (hazard assessment)
    - Late(r) innovation: Experimental results
  - Information regarding the chemical production (PROCs)
  - Operational conditions (OCs)

Tested tools

- ECETOC TRA
- INTEGRA

- Application scenarios:
  - **BPA alternatives in polycarbonate used in reusable water bottles**
  - BPA alternatives in epoxy resins in paint

Early stage innovation

PC bottle production								
Human Health								Environment
CSs	PROC 6	PROC 8b	PROC 9	PROC 10	PROC 14	PROC 15	SSbD Score	ERC 5
BPA	1	1	1	0	1	1	1	0
BPAP	1	1	1	0	1	1	1	0
Isosorbide	1	3	3	1	3	3	2	3

Late(r) stage innovation

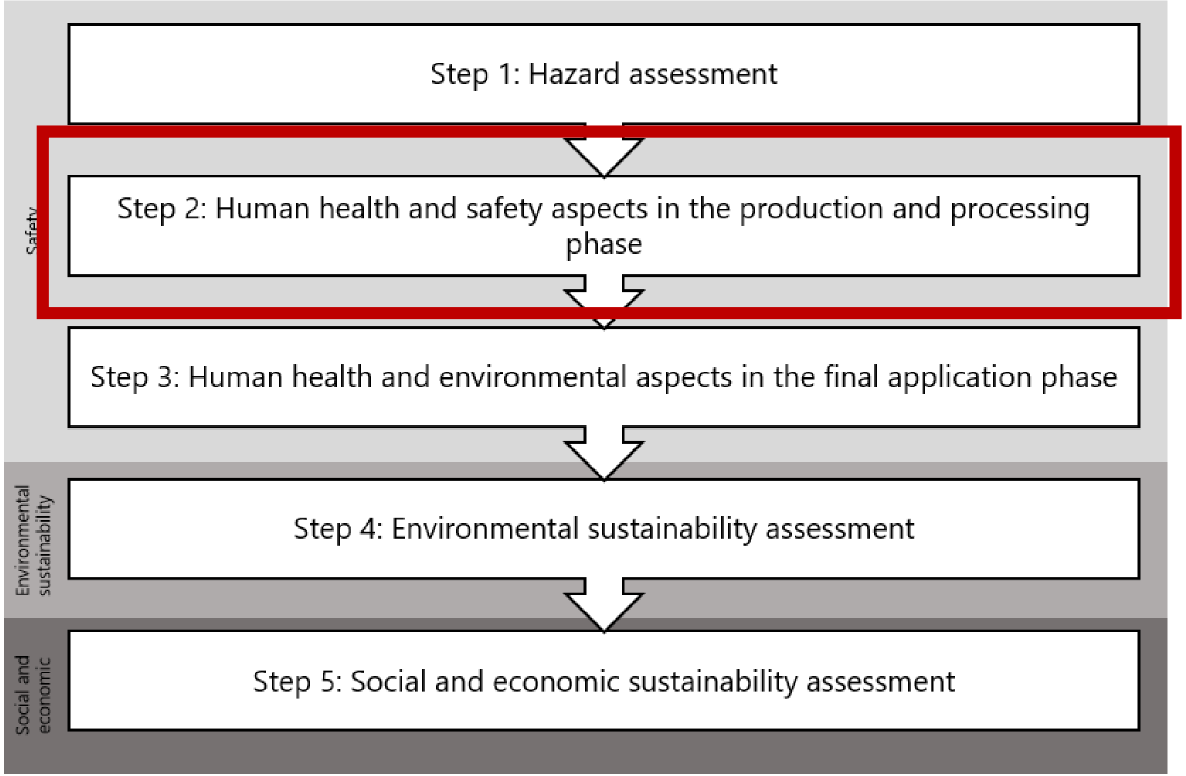
Production of PC Bottles								
Human Health								Environment
CSs	PROC 6	PROC 8b	PROC 9	PROC 10	PROC 14	PROC 15	SSbD Score	ERC 5
BPA	1	1	1	1	1	1	1	2
BPAP	1	1	1	0	1	1	1	0
Isosorbide	3	3	3	3	3	3	3	3

Step 2: exposure and risk during processing and production

- SSbD scores during the early stages are lower compared to those in the later stages
  → ECETOC TRA can provide a conservative and basic exposure assessment

- Final results of exposure estimates and risk can be influenced by the type of tool or data used for their calculation

- Many of the QSAR predictions were characterized with low reliability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Step 3: risk to consumers and the environment

- Requirements:
  - Specific application: reusable water bottle
  - Physicochemical, environmental fate and toxicological properties
    - Early innovation: QSAR results step 1 (hazard assessment)
    - Late(r) innovation: Experimental results

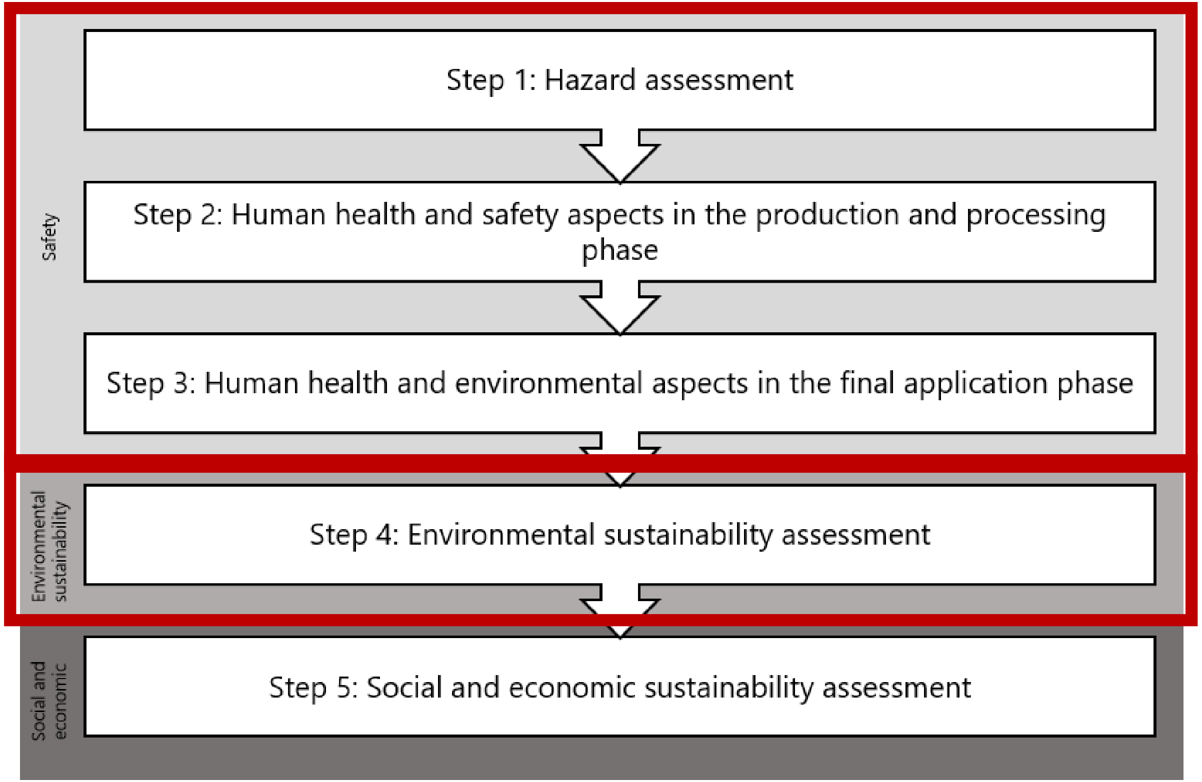
Tested tools

- INTEGRA
- Vermeer FCM

Set toxicological threshold → Predict exposure → Define risk

Step 3: risk to consumers and the environment

- Toxicological thresholds affect the final outcomes
- Difference between between risk in early and late innovation due to lower TDI values in late innovation
  - The application of QSAR predictions should be approached conservatively when there is no available data.
- Approach raises concerns about the accuracy and reliability of results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Method	Impact categories	Results
GaBi: Screening LCA	• Acidification • Climate change • Ecotoxicity • **Eutrofication** • Human toxicity (cancer, non-cancer) • **Land use** • Ozone depletion • Particulate matter • Photochemical ozone transf. • Fossil based resources • **Mineral and metals** • **Water use**	• Solvent type in the production is heavily dominating in most of the impact categories • Higher impacts in four impact categories for Isosorbide (biobased chemical)
QuasaLCA: specific information on production (based on ecoinvent v3.8 and published literature)	• Acidification • Climate change • Ecotoxicity • Land use (urban) • Land use (agriculture) • Particulate matter • Water use	• Isosorbide plastic bottle has a lower EF • Dishwashing is a major contributor to overall EF • For BPA, production contributes significantly

Step 4: environmental sustainability assessment

- Conflicting results need to be further studied

- lack of data (LCIs) of chemicals
  - Large databases such as Ecoinvent only have a fraction of processes available for chemical production
  - Several methods to generate LCIs for chemicals have been developed but the quality of the result can vary widely

Some final thoughts

- By conducting the case study we have a better understanding of the applicability of different tools for SSbD assessments

- Most tools are easy to use, but the results are difficult to interpret
- Data to run the tools is limited
- How to balance complexity of chemical production and use vs. feasibility of the assessment

- Some other aspects should be addressed:
  - Uncertainty and reliability of the models and data
  - Incorporation of circular economy considerations
  - Comparison of chemicals that exist on different development levels
  - …

The case-study team

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