From Complexity to Simplicity: Towards Streamlining Safety and Sustainability Assessments

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ABSTRACT / BACKGROUND

Assessments for Safety and Sustainability

- In line with recent frameworks, safety and sustainability performance needs to be assessed along the product life cycle and outcomes need to be quantitative to allow for aggregation into comprehensive evaluations of overall impact (e.g. climate, water consumption, etc.).
- While tools and approaches are available for SSbD assessments, their applicability and relevance regarding mixtures are hardly evaluated.
- ECETOC's work aims to provide safety input for multidimensional sustainability evaluations. As a first step, the comparative safety assessment of mixture is explored. (JRC 2022)

Comparative Safety Assessment for Mixtures

- A large portion of incremental innovations in the chemical industry comes from new mixtures.
- One of the key factors in the innovation process is whether the mixture is "safer" than its predecessor. To assess this, there should be a clear definition and evaluation criteria, which is not currently the case.
- Objective: Establish the feasibility and directional reliability of a comparative safety assessment of mixtures.

METHOD

Tool selection criteria

While there are many tools available for safety assessment, not all of them are suitable for life cycle oriented comparative safety assessment of mixtures. Therefore, we have defined the following criteria for selecting the appropriate tools:

- ✓ Safety: assessment should be risk-based (comparing hazard and exposure considerations), ideally following processes used in existing regulatory frameworks (e.g. REACH).
- ✓ Feasibility: input data must be readily available for a large number of chemicals and the tools themselves needs to utilize this input.
- ✓ Directional reliability of comparison: Uncertainty of outcome needs to be established in view of uncertainty of input data, input data needs to have the same information value (compare apples with apples).

As a starting point the task force has identified the freely available **ProScale** tool and its environment safety module **ProScaleE**, hosted by IVL, as suitable for comparing mixtures with regards to chemical safety along the product life cycle. (Lexén, J, et al. 2021; IVL 2025)

Criteria:	ProScale tool:
Risk based assessment →	Accounting for hazard (H) and exposure (E) via their respective scores.
Quantifying degree of safety along life cycle →	Safety score (S) $S = H \times E$
Easily available input: substance hazard & properties →	H-Phrases, vapor pressure, biodegradability (from safety data sheets)
Easily available input: use / exposure →	REACH exposure info: PROCs, SPERCs (from REACH use maps)
Useful results in life-cycle assessment →	Functional unit is the basis for assessment

JOINT IVL / ECETOC REVIEW OF HAZARD SCORES

Hazard Scores – Human Health (ProScale): No need for change – IVL and ECETOC find current scores appropriate.

Hazard Scores – Environment (ProScaleE): Need for alignment with CLP, map hazard scores to hazard bands

ProScaleE Hazard Score assignment vs CLP

	ProScaleE	CLP
Spacing of hazard classes	H412 to H411: decadic; H411 to H410: none	Decadic, a factor of 10
Weight M-factor	3 or 3.33	Decadic, a factor of 10
Safety net H413	Hazard score = 10	No hazard assigned
Rapid degradability	Hazard score assigned **w/o** distinction	H-phrase **depends on** degradability

Need for alignment with CLP

Hazard Scores: Unambiguous mapping to effect bands

Hazard Class / Effect Band (mg/L)*	Hazard Score
PBT, vPvB, PMT, vPvM	100 000
ED Cat 1	100 000
ED Cat 2	10 000
10^{-6} - 10^{-5}	100 000
10^{-5} - 10^{-4}	10 000
10^{-4} - 10^{-3}	1 000
10^{-3} - 10^{-2}	100
10^{-2} - 10^{-1}	10
10^{-1} - 1	1
1 - 10	0.1

One effect band – one hazard score

Result: Mapping of Hazard Scores to Hazard Classes taking degradability into account

Hazard Class	M-Factor	Hazard Score	
		Rapidly degrading	Not rapidly degrading
PBT, vPvB, PMT, vPvM		100 000	100 000
ED Cat 1		100 000	100 000
ED Cat 2		10 000	10 000
H400*	1000	10 000	1 000
H400*	100	1 000	100
H400*	10	100	10
H400*	1	10	1
H410	1000	100 000	10 000
H410	100	10 000	1 000
H410	10	1 000	100
H410	1	100	10
H411	n.a.	10	1
H412	n.a.	1	0.1
H413	n.a.	0.1	0.1

NEXT STEPS

- Collect suitable pairs of products for comparative safety assessments.
- Conduct a series of case studies of comparative safety assessments using ProScale.
- Define the interpretation criteria of the results: Under which conditions is the statement, "Product A is safer than Product B" correct. Define conditions for clearly distinguishing two mixtures/products based on the safety metric obtained from ProScale/ProScaleE.
- Find a method to weight human health and environment scores to obtain a single result for a mixture.

Online Poster

References

JRC, Joint Research Centre. (2022) Safe and Sustainable by Design chemicals and materials - Review of safety and sustainability dimensions, aspects, methods, indicators, and tools. JRC127109

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