MCDA – a Valuable Approach for the Final Evaluation within the SSbD Framework?

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Safe and Sustainable by Design

- Working definition of SSbD:
  - no (or low) hazards according to Article 57 of REACH: PBT, vPvB, human toxicity etc.
  - no (or low) Global Warming Potential and ODP

Multi-Criteria Decision Analysis

Environmental Science & Technology

Article

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Combining in Silico Tools with Multicriteria Ar… Assessment of Hazardous Chemicals: A Case … Decabromodiphenyl Ether Alternatives

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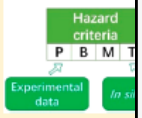
Supporting Information

ABSTRACT: Alternatives assessment is applied for minimizing the risk of unintentionally replacing a hazardous chemical with another hazardous chemical. Central challenges are the diversity of properties to consider and the lack of high-quality experimental data. To address this, a novel alternatives assessment procedure was developed based on in silico data and multicriteria decision analysis (MCDA) methods. As a case study, 16 alternatives to the flame retardant decabromodiphenyl ether were considered. The hazard properties included persistence (P), bioaccumulation potential (B), toxicities (T), and mobility in water (M). Databases were consulted and 2866 experimental data points were collected for the target



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Article

Combining *In Silico* Tools with Multicriteria Analysis for Alternatives Assessment of Hazardous Chemicals: Accounting for the Transformation Products of decaBDE and Its Alternatives

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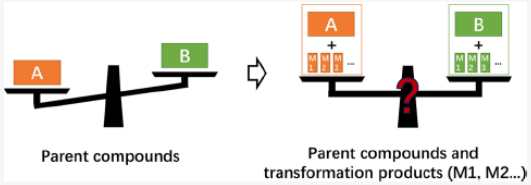
ABSTRACT: Transformation products ought to be an important consideration in chemical alternatives assessment. In this study, a recently established hazard ranking tool for alternatives assessment based on *in silico* data and multicriteria decision analysis (MCDA) methods was further developed to include chemical transformation products. Decabromodiphenyl ether (decaBDE) and five proposed alternatives were selected as case chemicals; biotic and abiotic transformation reactions were considered using five *in silico* tools. A



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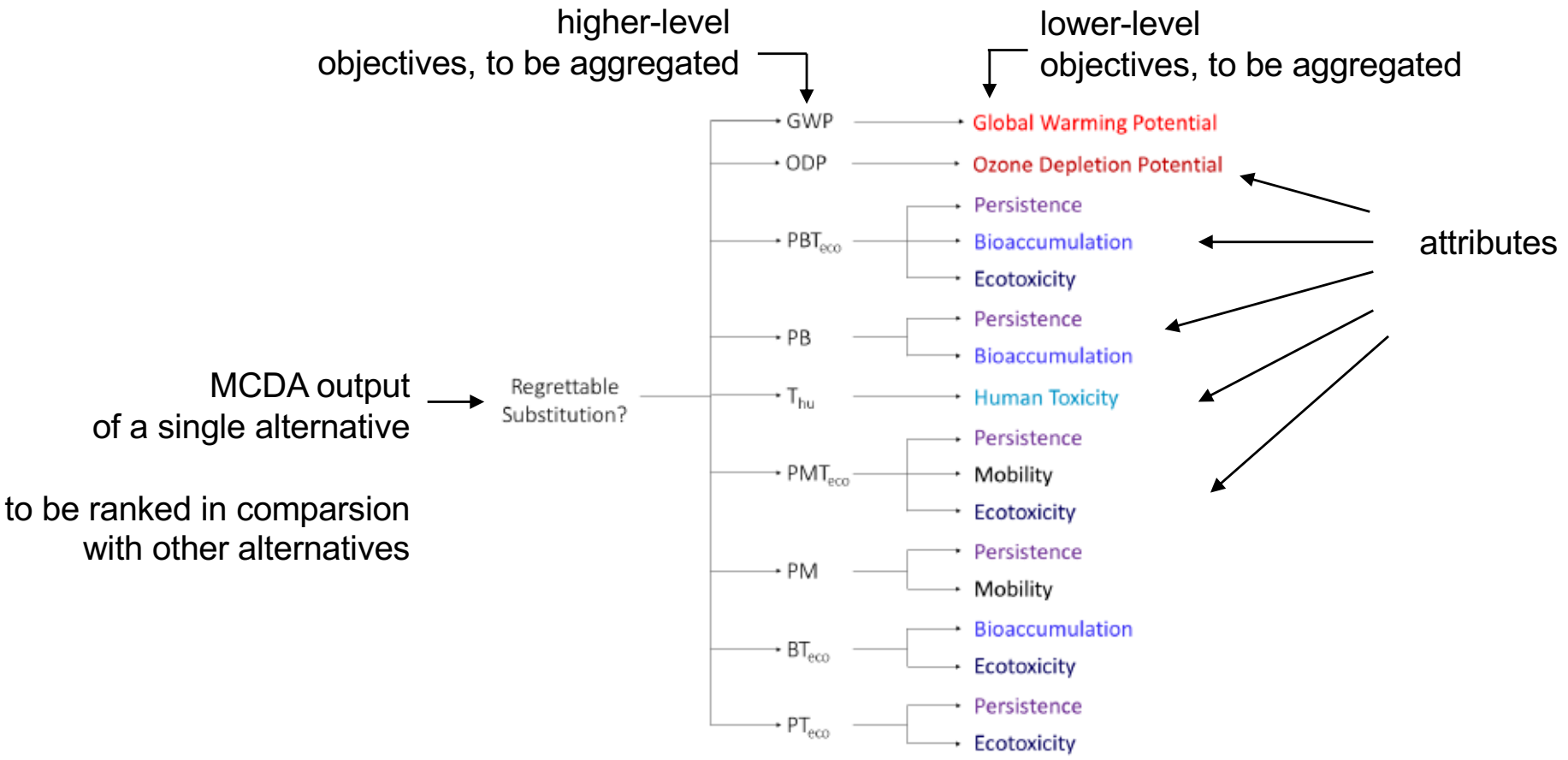
Multi-Criteria Decision Analysis



R. London et al. (2024), https://doi.org/10.26434/chemrxiv-2024-dmb5d

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Multi-Criteria Decision Analysis

- Alternatives are characterized by **attributes.**
- **Objectives** describe wanted/unwanted properties of these attributes.
- Objectives should be independent of one another.
- For each alternative, objectives are **aggregated** to give a score or an **MCDA output** of the alternative.
- Alternatives are **ranked** by their MCDA outputs.

MCDA Parameters

- **Value function** for scaling the properties of attributes
- **Weights** of different attributes in aggregation
- **Type of aggregation:** additive, minimum, …

- Absolute **reference points** for MCDA output

R. London et al. (2024), https://doi.org/10.26434/chemrxiv-2024-dmb5d

Our Approach

- A test set of **256 hypothetical chemicals** with diverse combinations of four hazards (= attributes):
- Persistence, bioaccumulation potential, ecotoxicity, human toxicity
- Each attribute: low, medium, high, very high.
- Assessment according to Article 57 of REACH shows: 148 substances have SVHC properties (substances of very high concern)

R. London et al. (2024), https://doi.org/10.26434/chemrxiv-2024-dmb5d

MCDA and Other Methods vs. Article 57 of REACH

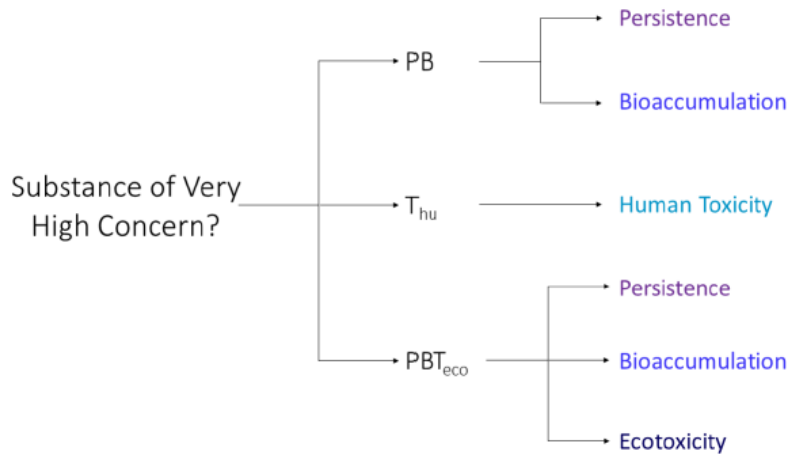
- Apply a range of methods (Cradle-to-cradle, GreenScreen, MCDA, ...) to the 256 test chemicals

- Outcome: none of the methods can capture the decision logic of Article 57: the classification of 148 SVHCs vs. 108 non-SVHCs cannot be reproduced

R. London et al. (2024), https://doi.org/10.26434/chemrxiv-2024-21mv3

Aligning MCDA with Article 57

- A simplified decision logic reflecting Article 57:



objectives are not independent

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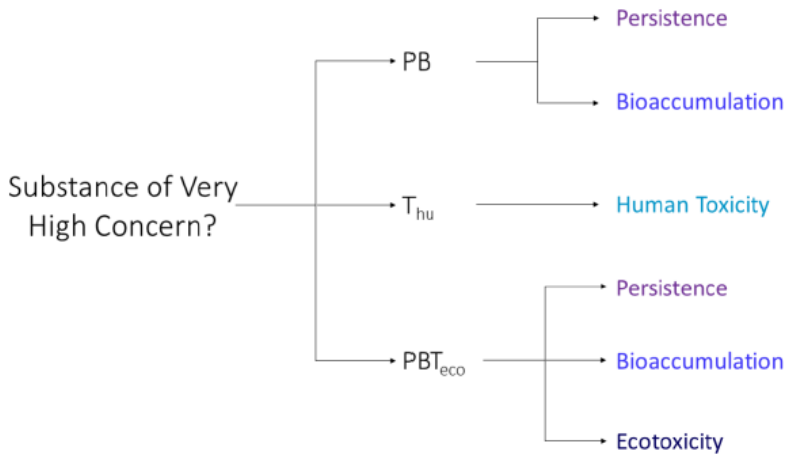
Aligning MCDA with Article 57

- Correct classification of 148 SVHCs vs. 108 non-SVHCs?



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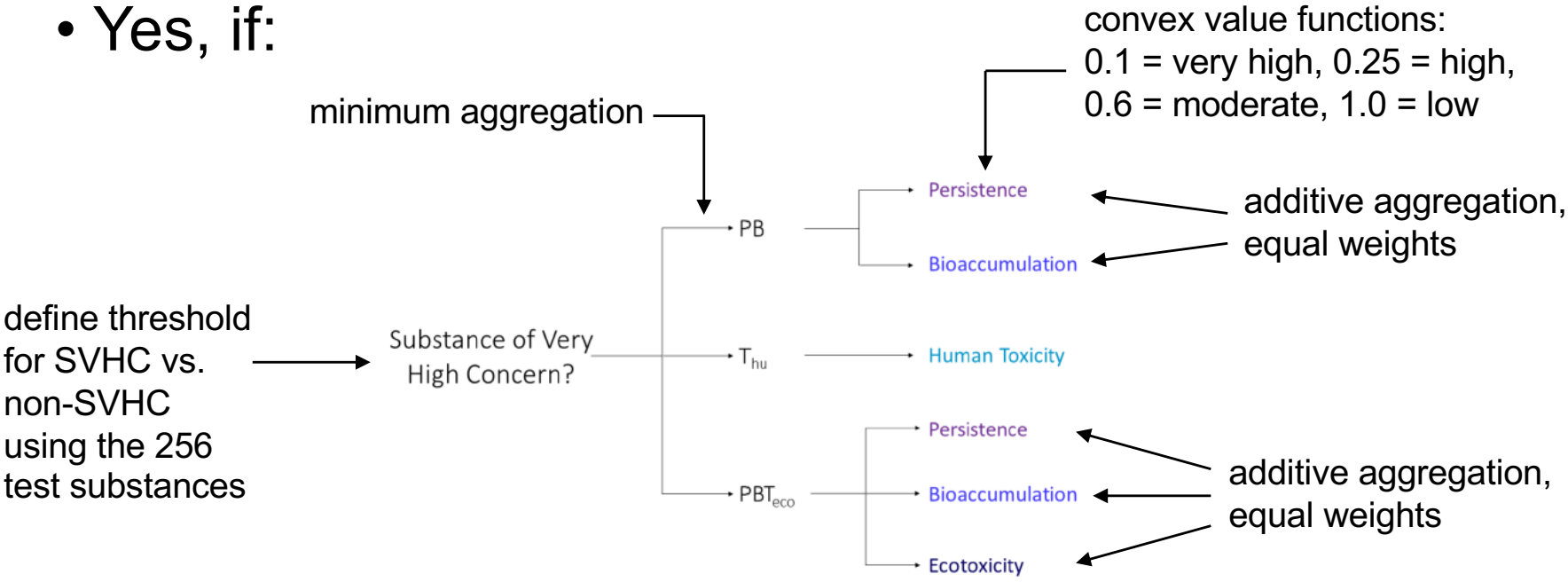
Aligning MCDA with Article 57

- Correct classification of 148 SVHCs vs. 108 non-SVHCs?
- Yes, if:



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Conclusions: Before Applying MCDA …

- … define the **decision logic**, including normative values
- … gather all **input data** describing the attributes of all alternatives (i.e., chemicals)
- … set the **MCDA parameters** according to the decision logic
- And: do not overestimate the power of a method

R. London et al. (2024), https://doi.org/10.26434/chemrxiv-2024-dmb5d

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