Finnish Institute of
Occupational Health

MCDA-assisted chemical alternatives assessment based on input data generated using the SSbD toolbox

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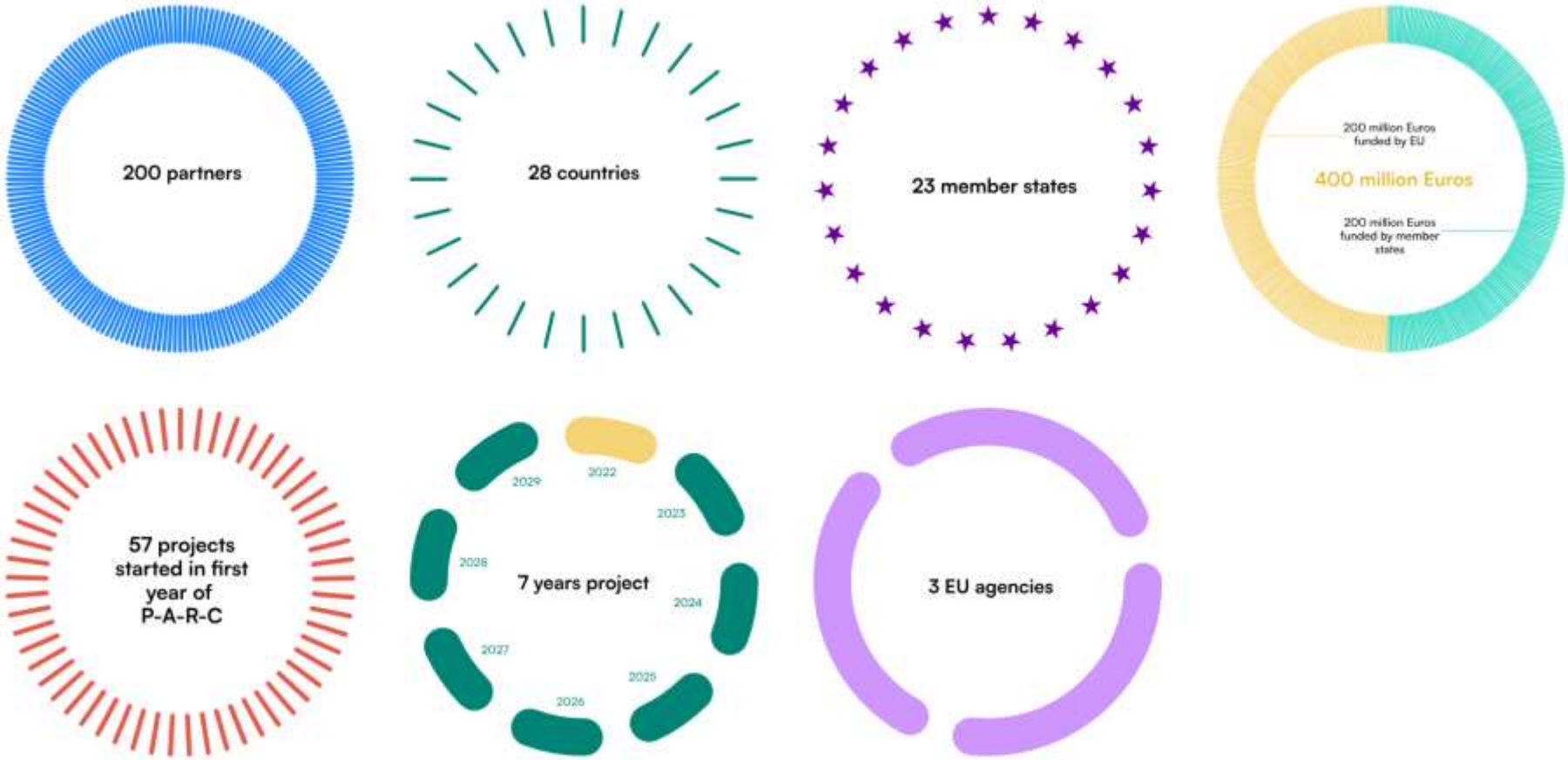
Partnership for the assessment of risks from chemicals (PARC)



Source: eu-parc.eu/parc-figures

Safe and Sustainable by Design – SSbD

- A prevention approach within the EU Chemicals Strategy for Sustainability
- An approach for evaluating and developing new chemicals and materials, and for evaluating existing ones

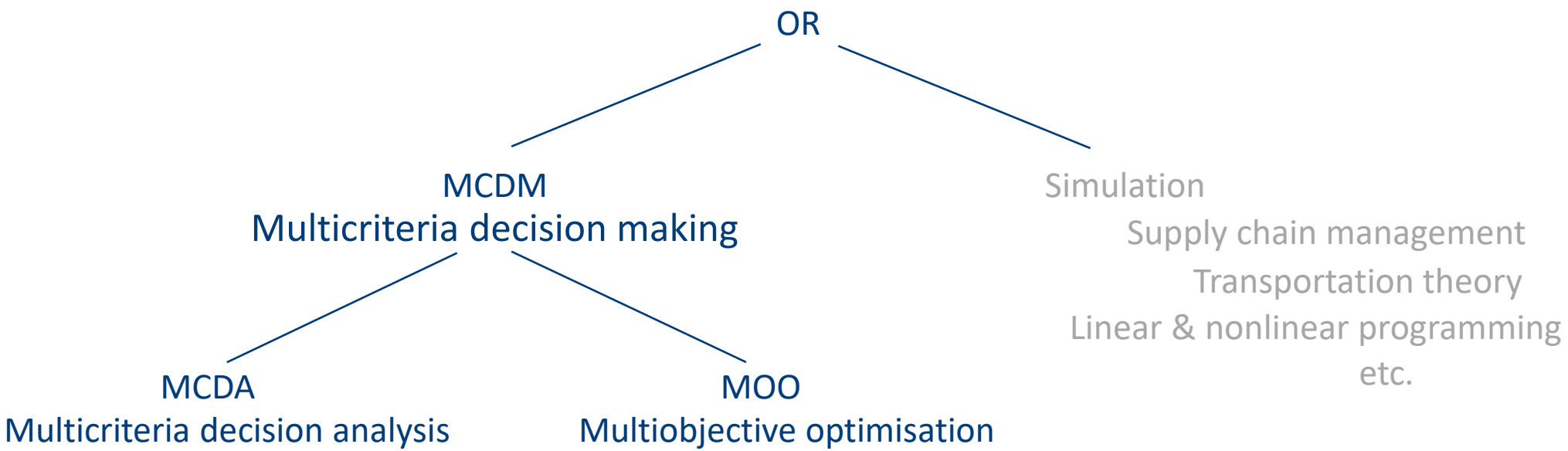
SSbD toolbox

- “The goals of the toolbox are to provide:
- → A structured inventory and overview of tools suited for SSbD assessment and (re-)design;
- → Structured workflows for applying the tools to answer SSbD assessment and (re-)design questions;
- → An evaluation and decision-support approach to support interpretation and follow-up (re-)design actions;
- → A clear connection with the commercial developmental stages of a chemical or material;
- → Incorporating the foreseen production, use conditions and end-of-life of the chemical, material or product.”

Source: parc-ssbd.eu

Chemical substitution as a case

Decision science as part of operations research (OR)



MCDA is a decision-making process with applied mathematics

MCDA is used when there are:

- Predefined set of decision alternatives
- Multiple decision criteria that must be considered
- When human cognition is faced with a complex decision problem, and welcomes decision aid to make a legitimate decision, that is transparent, traceable, and reproducible

MCDA includes:

- Trade-offs between decision criteria
- Sometimes, multiple decision-makers and stakeholders (group decision-making)
- Identification of the best alternative, or the most satisfying one

Steps in MCDA

1. Establishing the decision context
2. Identifying the decision alternatives
3. Identifying the objectives and criteria
4. Assigning scores to each alternative for every criterion
5. Assigning weights for each of the criteria
6. Deriving overall value of the alternatives by combining weights and scores
7. Examining the results
8. Conducting a sensitivity analysis

Three basic elements of MCDA

- Decision matrix (also known as performance matrix or evaluation matrix)

Top four solvents of the ranking in benzene replacement					
Solvent	Parameters involved in the decision				
	Solubility			Toxicity	Cost
	Dielectric constant	Dipole moment (D)	Solubility parameter ENT (kcal/mol)	Oral LD50 (mg/kg)	Bulk cost (£/kg)
Benzene*	2,27	0	0,111	930	1,68
Ideal solvent	2,27	0	0,111	5000	1
Toluene	2,38	0,4	0,099	5000	1,23
Xylene	2,6	0,3	0,123	4300	1,9
1.1.2.2-Tetrachloroethylene	2,28	0	0,043	2629	0,9
1.4-Dioxane	2,2	0,4	0,164	5700	2,03

Source: Perez–Vega et al. (2011)

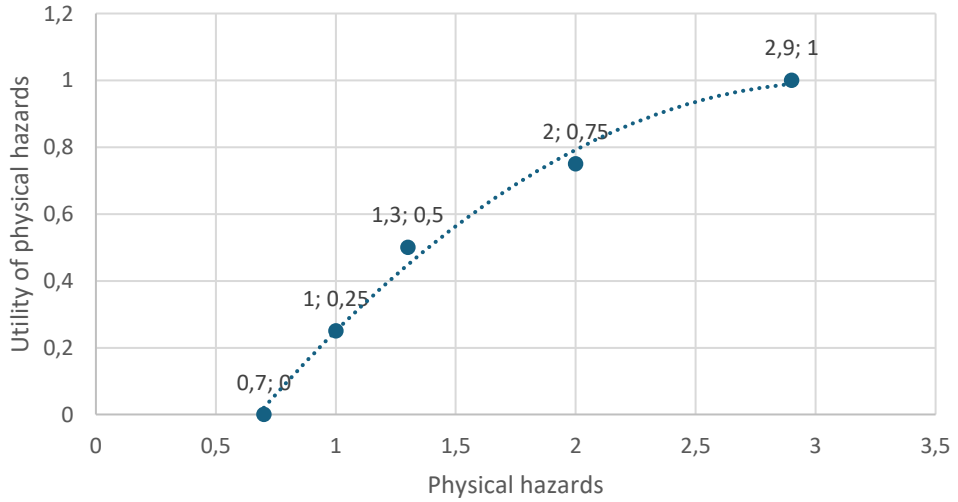
- Weighting method
- Aggregation method

Four categories of MCDA methods

Method family	Well known methods of the family
Multiattribute utility/value theory	MAUT/MAVT
Outranking methods	ELECTRE, PROMETHEE
Pairwise comparison methods	AHP, ANP
Distance based methods	TOPSIS

MAUT – finding the decision alternative with highest expected utility – two key parts

1) Assessment of attribute-specific (criterion-specific) utility functions



2) Aggregation of overall utility

Additive MAU function

$$u(x^j) = \sum_i w_i u_i(x_i^j)$$

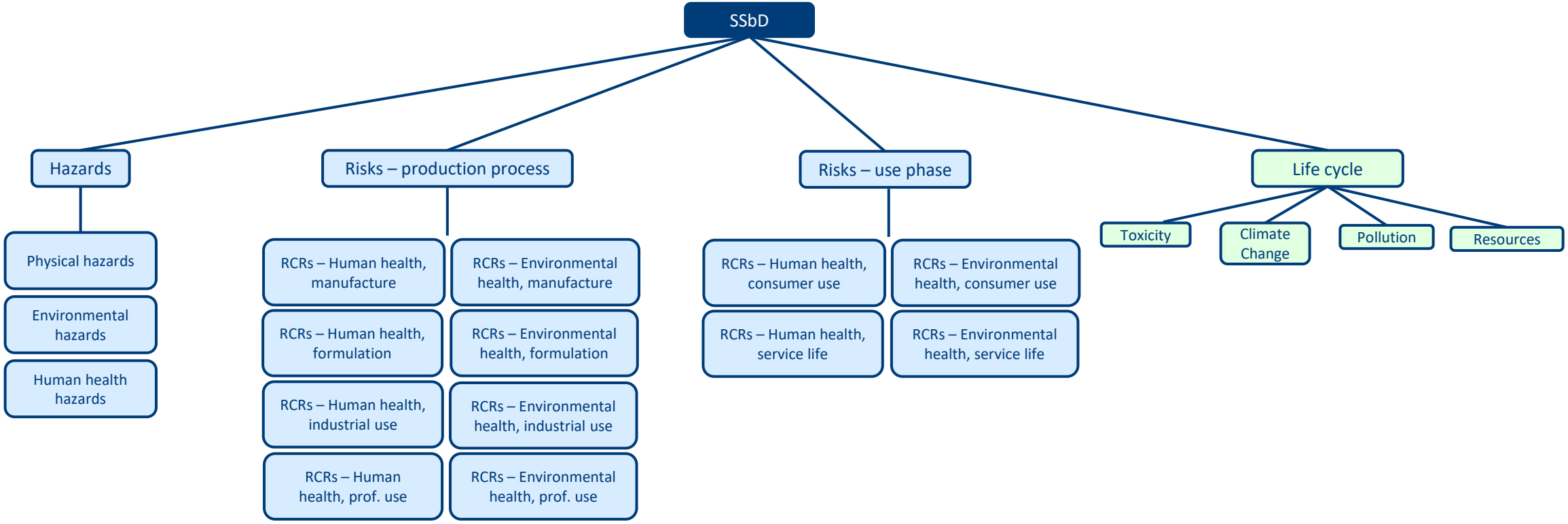
Multiplicative MAU function

$$u(x) = \frac{\prod_{i=1}^{n}[1 + k w_i u_i(x_i)]}{k} - \frac{1}{k}$$

Other utility functions do exist, too

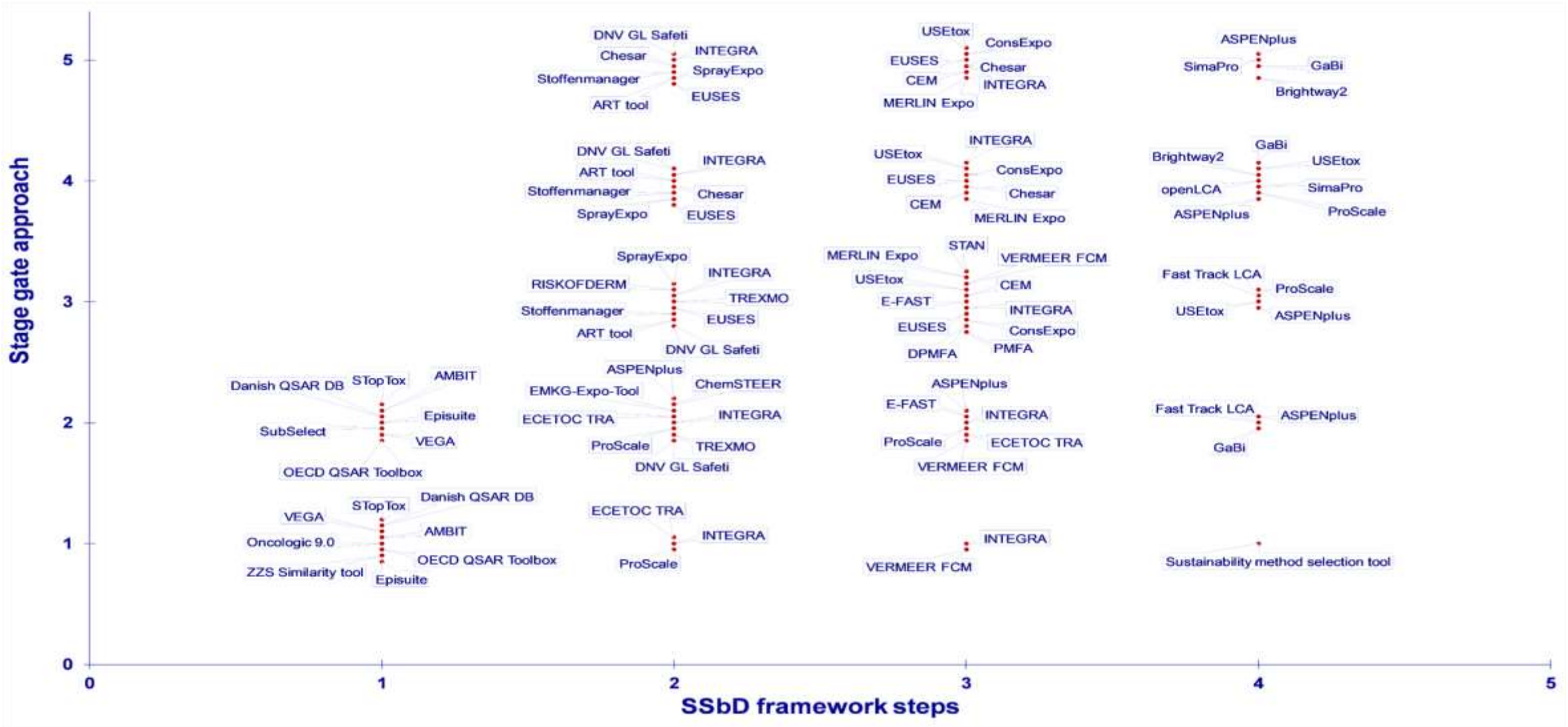
The SSbD assessment criteria

FIOH chemical industry case study version



RCR = risk characterization ratio, continous measurement criteria

Input data from the SSbD toolbox – the tools



Spyros Karakitsios, Aristotle University of Thessaloniki

Our case study with Finnish chemical industry

Our aim:

- To find the most suitable substitute chemical for our industrial partner
- To get use case experience for the SSbD toolbox development
- To explore MCDA’s potential in streamlining chemical product development
- To gain more insight into a MAUT process with incomplete information and the multiplicative model
- Possibly a comparison between MAUT and heuristics

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Thank you!

More information ↓

Lantto, E. (2025). MCDA applications in chemical alternatives assessment: a narrative review. Environ Syst Decis 45, 50.