



Predictive LCSA Framework for Lubricants within SSbD: Linking Environmental (LCA) and Socioeconomic (LCC, S-LCA, CRM, SVHC) Dimensions across Four Use Cases

GreenDeLTa

Jonas Hoffmann, Max F. Bringmann, A. Hamed

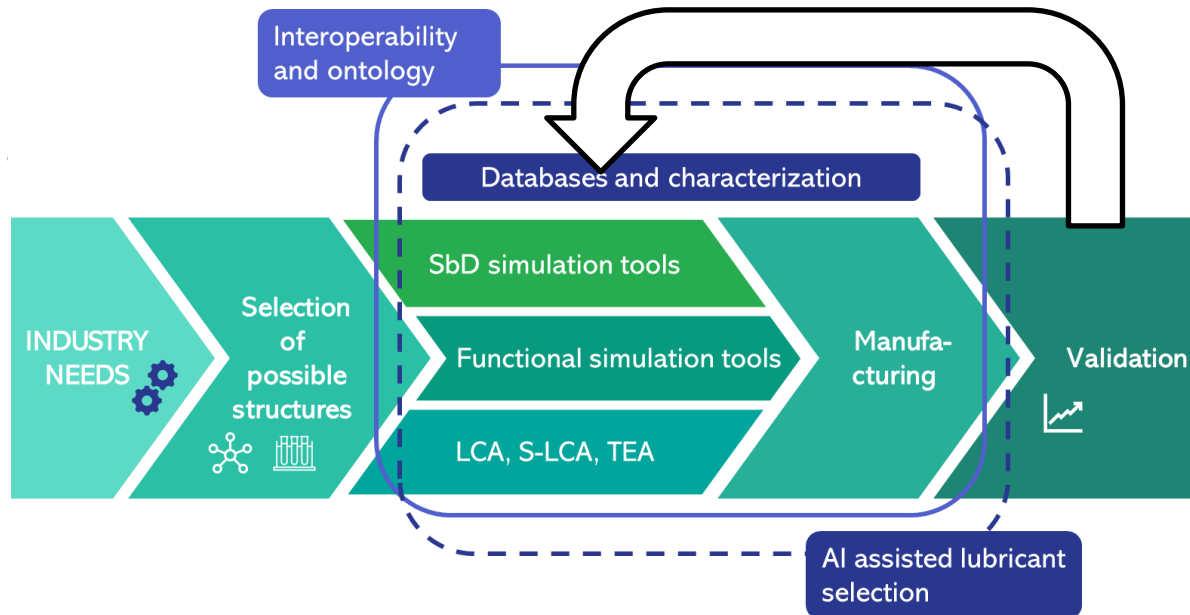


SETAC Europe 27th, LCA Symposium, Brugge

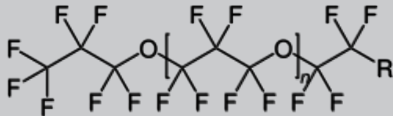
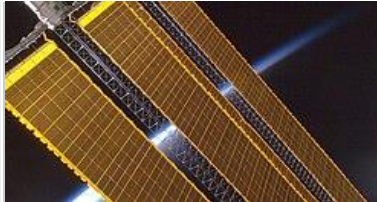
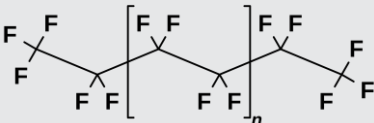
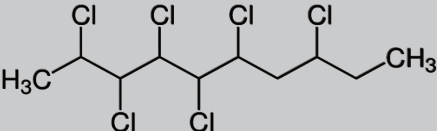
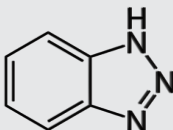
The SiToLub Project

SITOLUB - SIMULATION TOOLS FOR THE DESIGN OF SAFE AND SUSTAINABLE LUBRICANTS

HORIZON Research and Innovation Action:
Computational models for the development of safe and sustainable by design chemicals

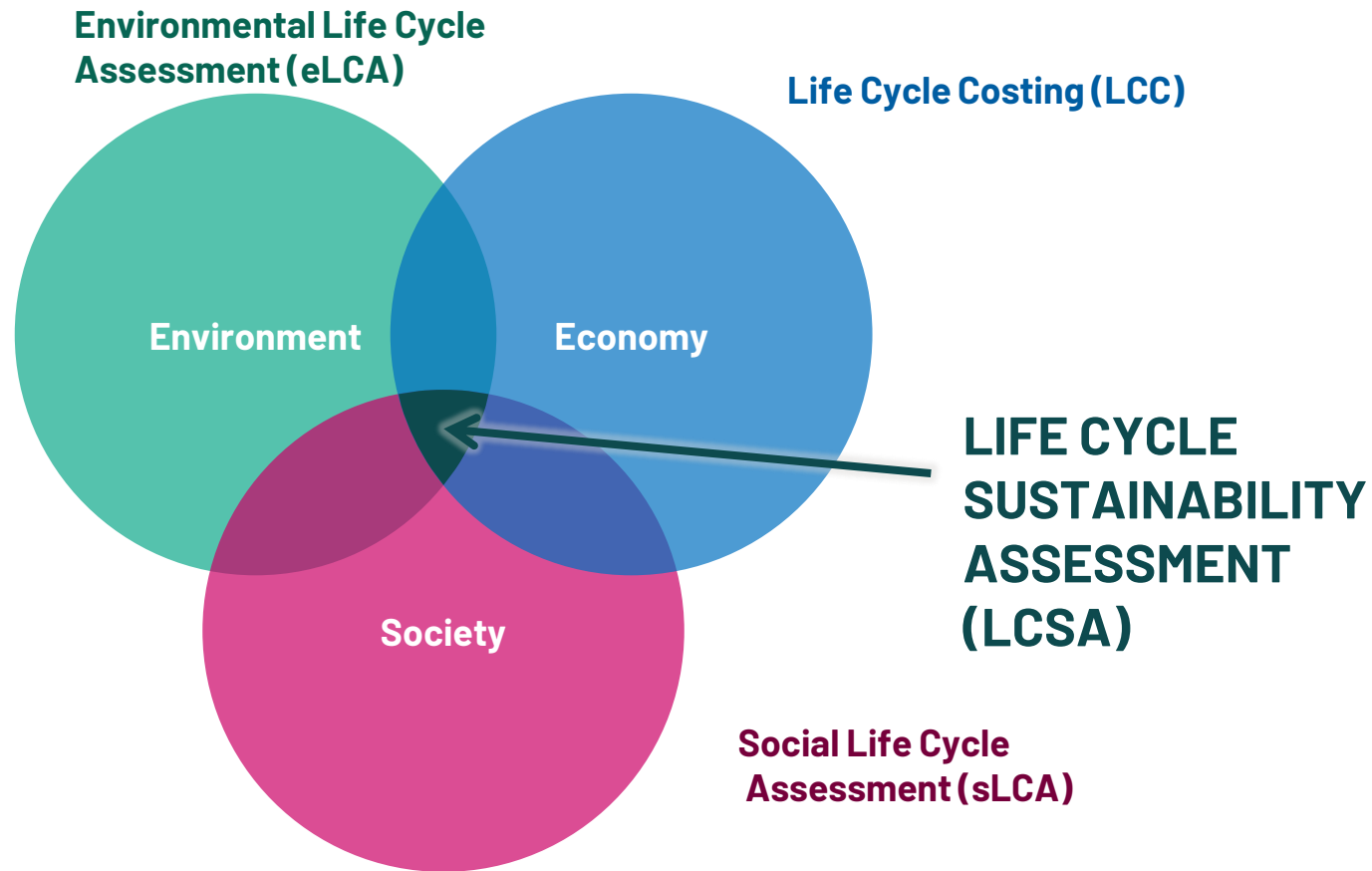


SiToLub: Use Cases

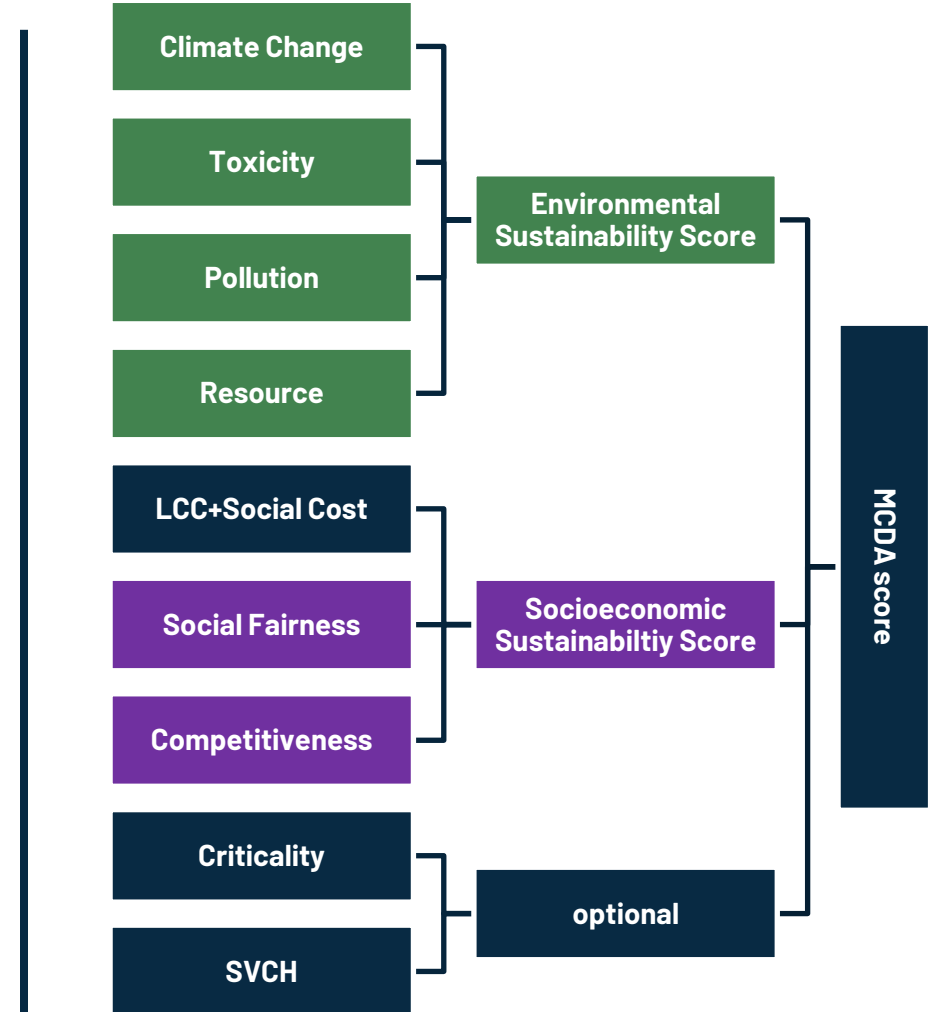
Use Case	Application		Issue
PFAS: PFPE 	Base oil		- Fugitive HFCs in production - Extremely persistent - Relying on CRM (CaF₂)
PFAS: PTFE 	Antiwear additive		- Same as above - PFAS as processing aids - Problematic EoL (PFAS)
Chlorinated paraffins (MCCP) 	Extreme-pressure additive		- Bioaccumulative and ecotoxic to aquatic - MCCPs (C14-17) fall under POP - Considered SVHC under REACH
Benzotriazole 	Corrosion inhibitor		- Persistent and highly mobile in water (PMT/vPvM concern) - Classified as acutely toxic if swallowed and harmful to aq.

Is a SSbD-inspired LCSA model capable to reflect those issues and predict alternatives?

LCSA and SSbD – it is a match

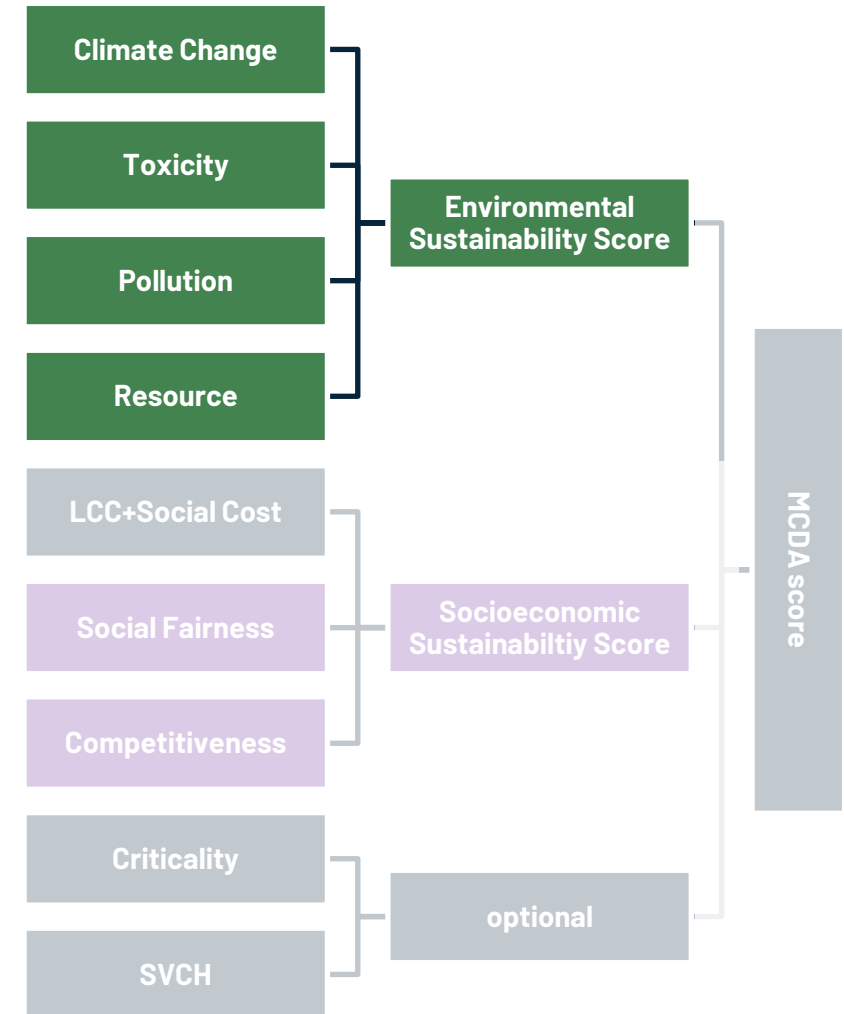
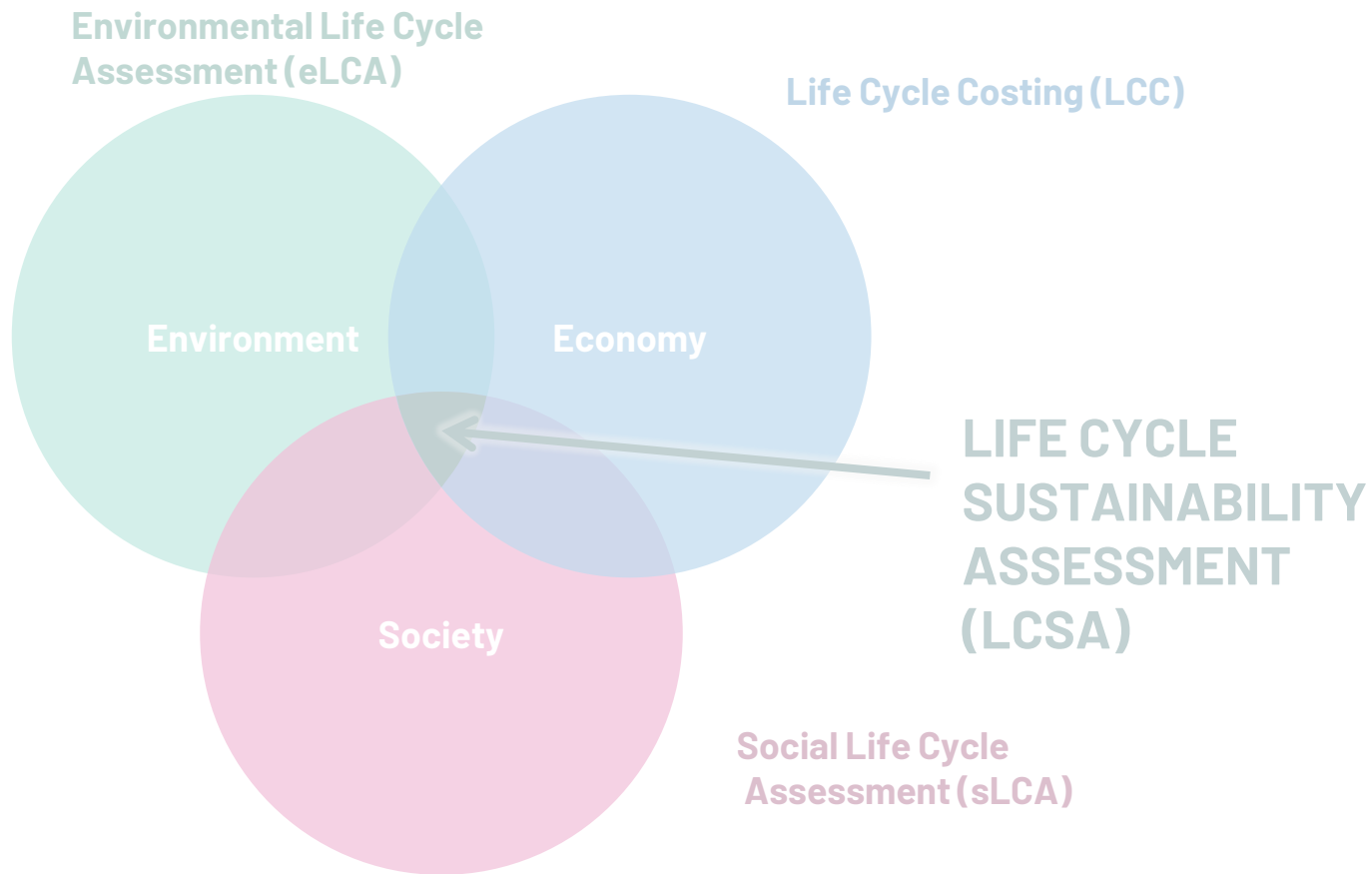


See ORIENTING (2020-2023) or UNEP (2011)

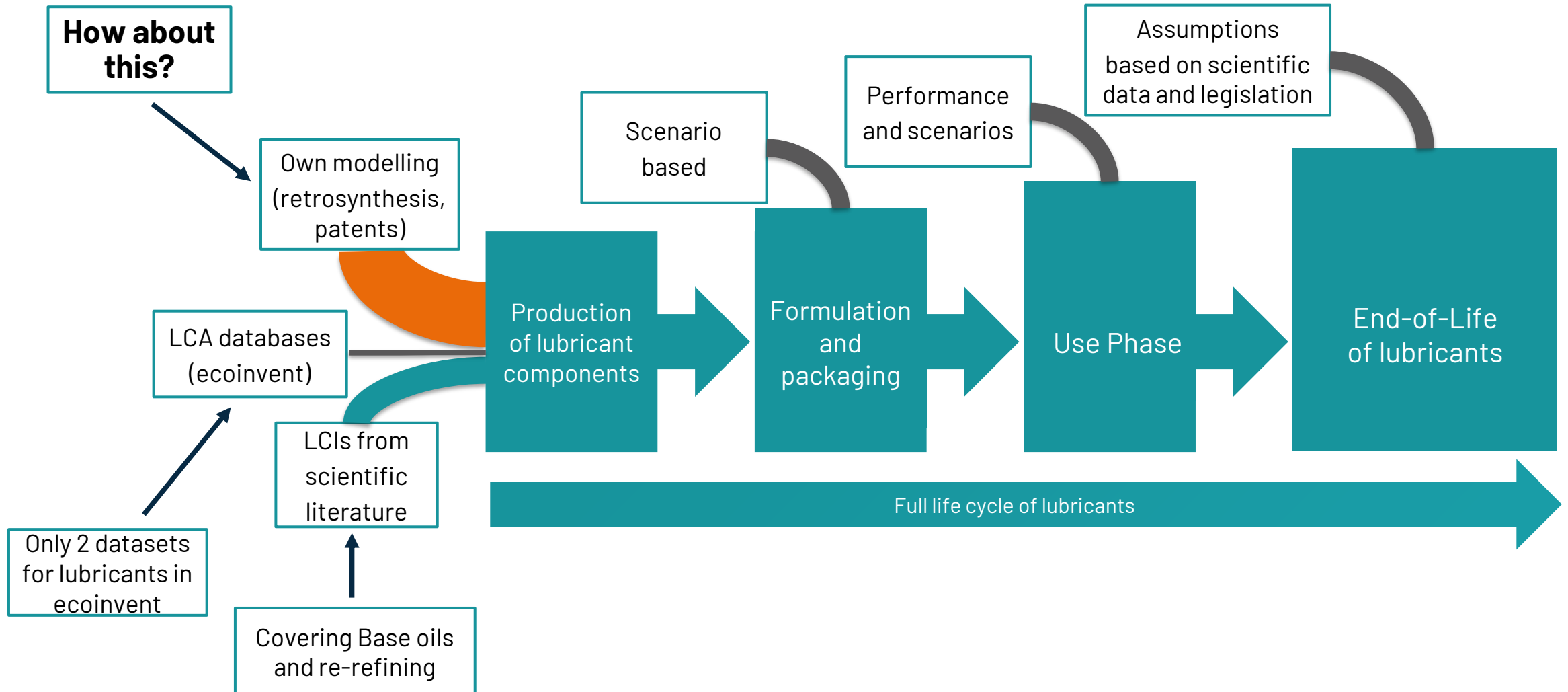


own work, SSbD framework (JRC, 2025)

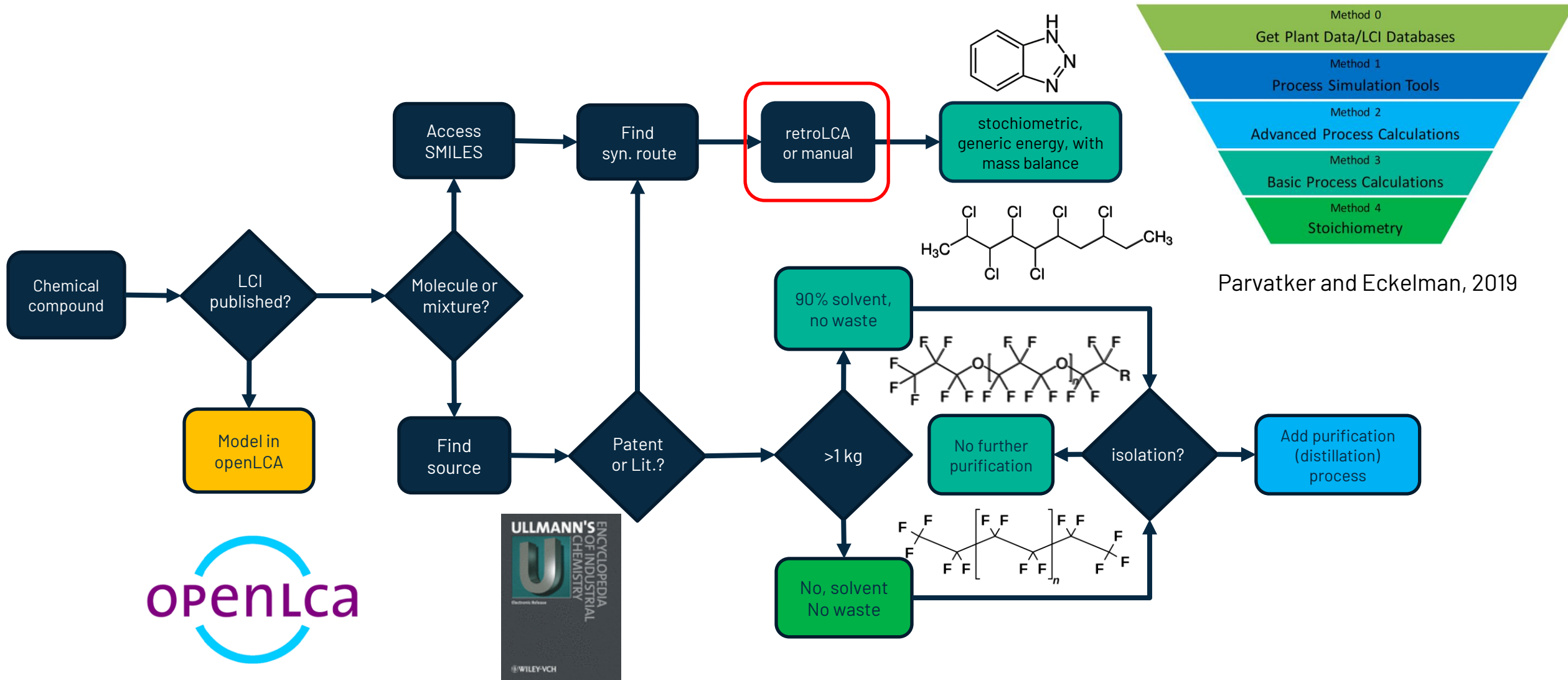
LCSA and SSbD – it is a match



Covering the full life cycle



LCA: Empirical workflow predicting inventories



openLCA becoming a chemist

LCA

2-ethylhexanal

General information - 2-ethylhexanal

- General information
- Used in processes
- Additional information 

CAS number 123-05-7

Formula

Synonyms Hexanal, 2-ethyl-; 2-Ethylhexaldehyde

Location  - none - 

General information | Flow properties | Additional properties

LCA

*2-ethylhexanal

General information - 2-ethylhexanal

- General information
- Used in processes
- Additional information

CAS number 123-05-7

Formula C8H16O

Synonyms Hexanal, 2-ethyl-; 2-Ethylhexaldehyde

Location  - none - 

General information | Flow properties | Additional properties

LCA

*2-ethylhexanal

Additional properties - 2-ethylhexanal

Key	Value
Connectivity	CCCCC(CC)C=O
Absolute-S	CCCCC(CC)C=O
InChI-String	InChI=1S/C8H16O/c1-3-5-6-8(4-2)7-9/h...
InChI-Key	LGYNIFWIKSEESD-UHFFFAOYSA-N

General information | Flow properties | Additional properties

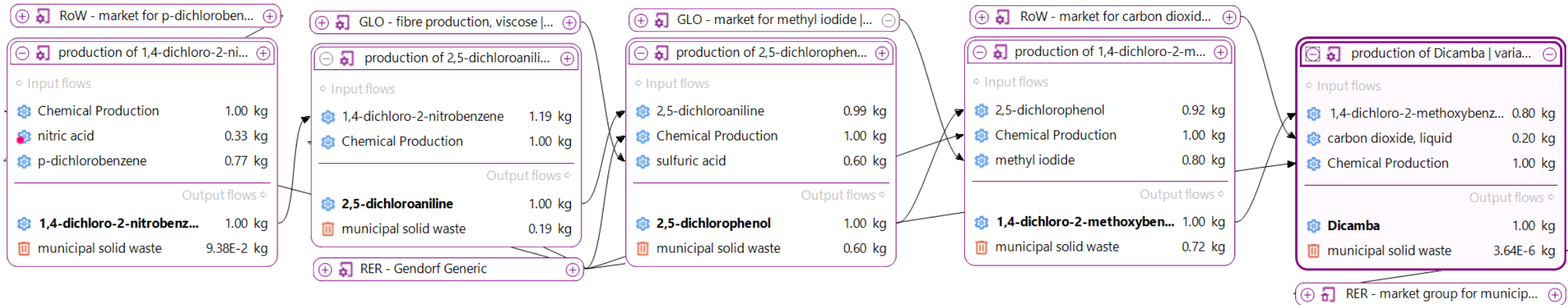
Matching name with PubChem

Adding SMILES to flows

openLCA becoming a real chemist



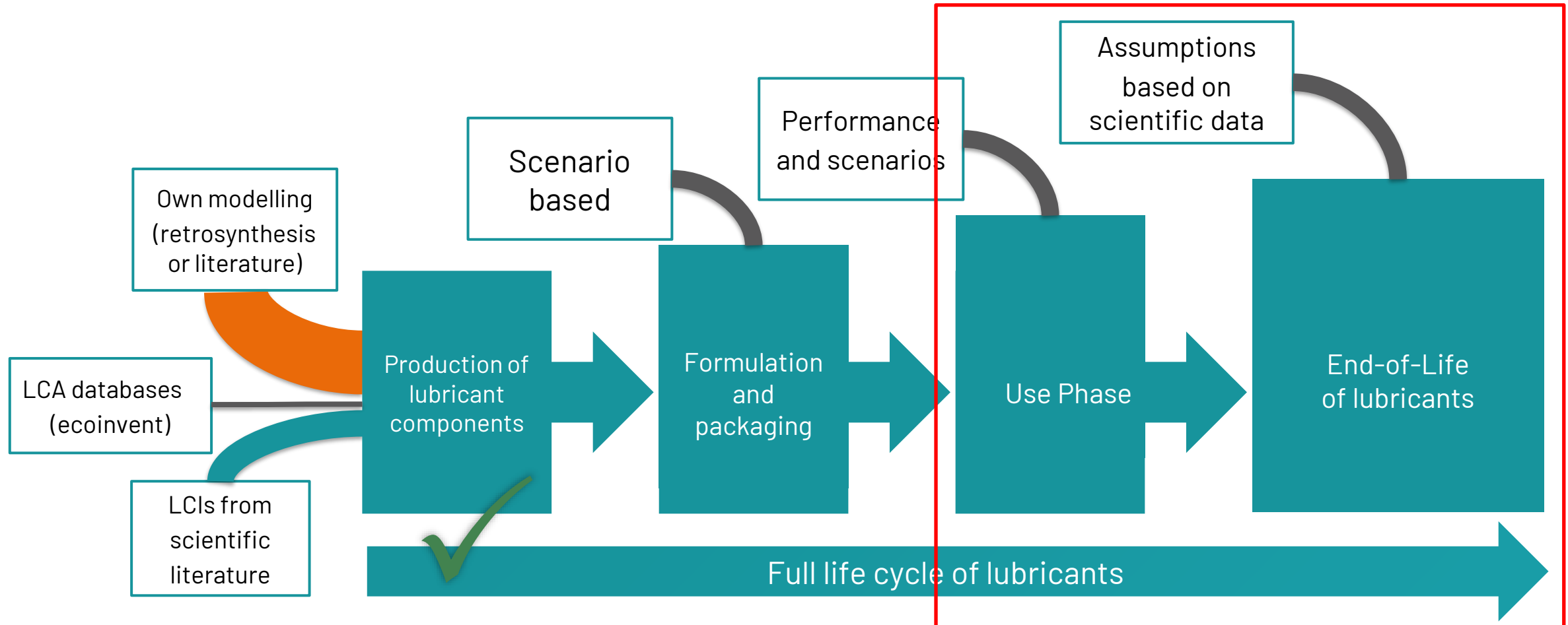
- We implemented retrosynthetic approaches in openLCA to build LCIs
- Based on SMILES codes, target chemicals are submitted to a retrosynthesis engine (e.g., AiZynthFinder or ASKCOS) and converted with RDKit/CIRPy



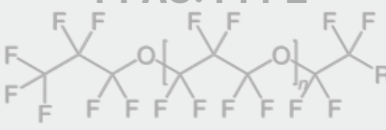
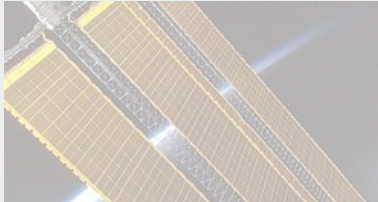
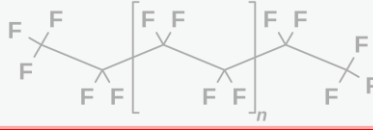
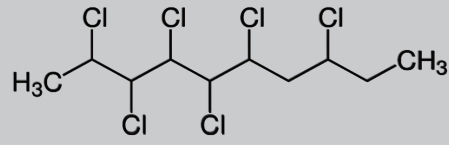
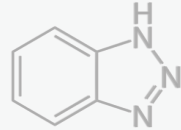
- retrolca automatically converts the selected pathway into an openLCA process network and connects it to the background database via SMILES

<https://github.com/GreenDelta/retrolca>

Covering the full life cycle

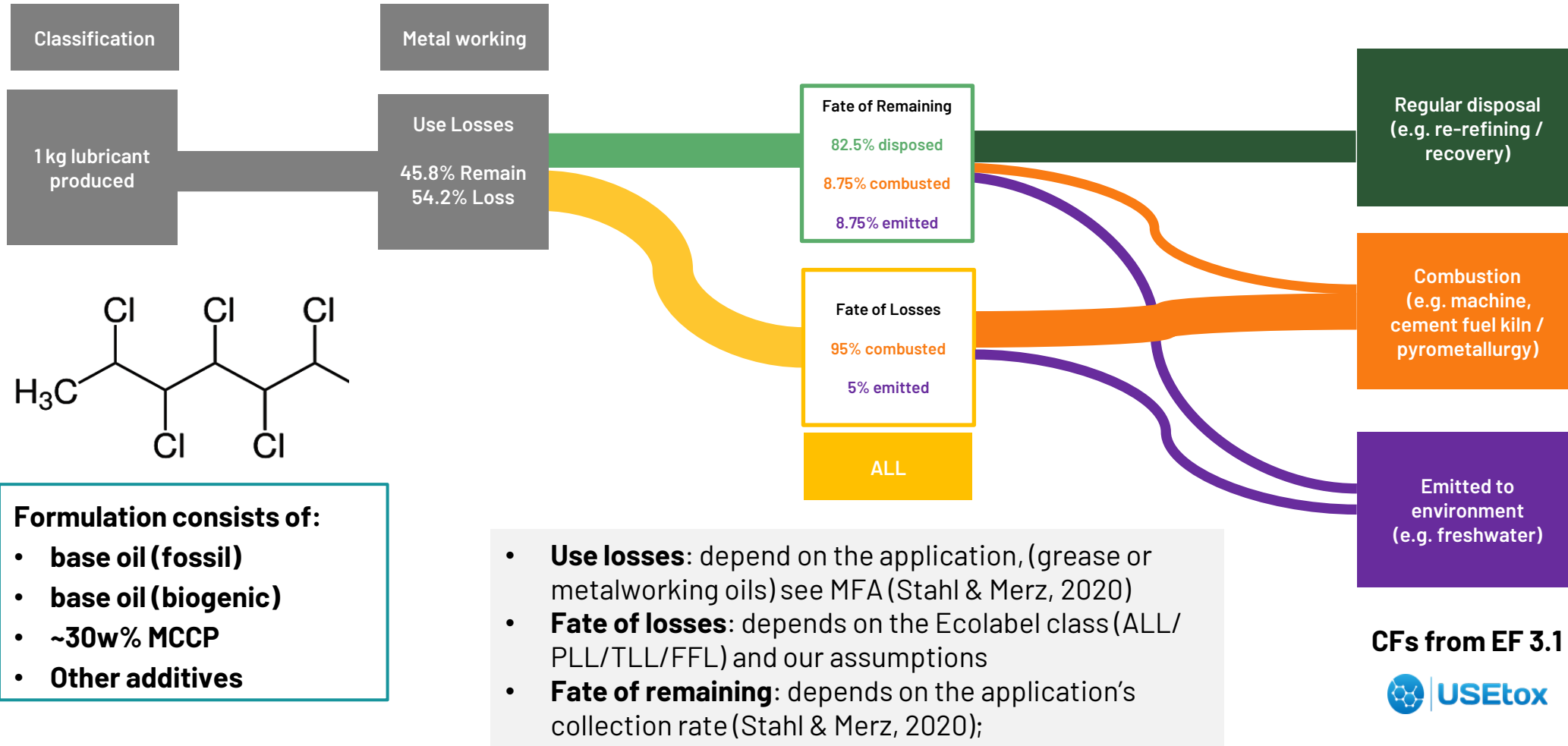


How to address the use phase?

Use Case	Application	Issue	Class
PFAS: PFPE 	Base oil	 - Fugitive HFCs in production - Extremely persistent - Relying on CRM (CaF₂)	Partial Loss
PFAS: PTFE 	Gears	 - Same as above - PFAS as processing aids - Problematic EoL (PFAS)	Filled for Life
Chlorinated paraffins (MCCP) 	Metal working fluid	 - Bioaccumulative and ecotoxic to aquatic - MCCPs (C14-17) fall under POP - Considered SVHC under REACH	Accid. Loss
Benzotriazole 	Corrosion inhibitor	 - Persistent and highly mobile in water (PMT/vPvM concern) - Classified as acutely toxic if swallowed and harmful to aquat.	Total Loss

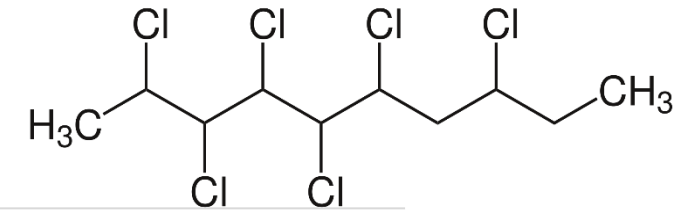
Lubricants represent an established technology: There is plenty of data for MFA of lubricants!

Predicting: Use Phase and EoL

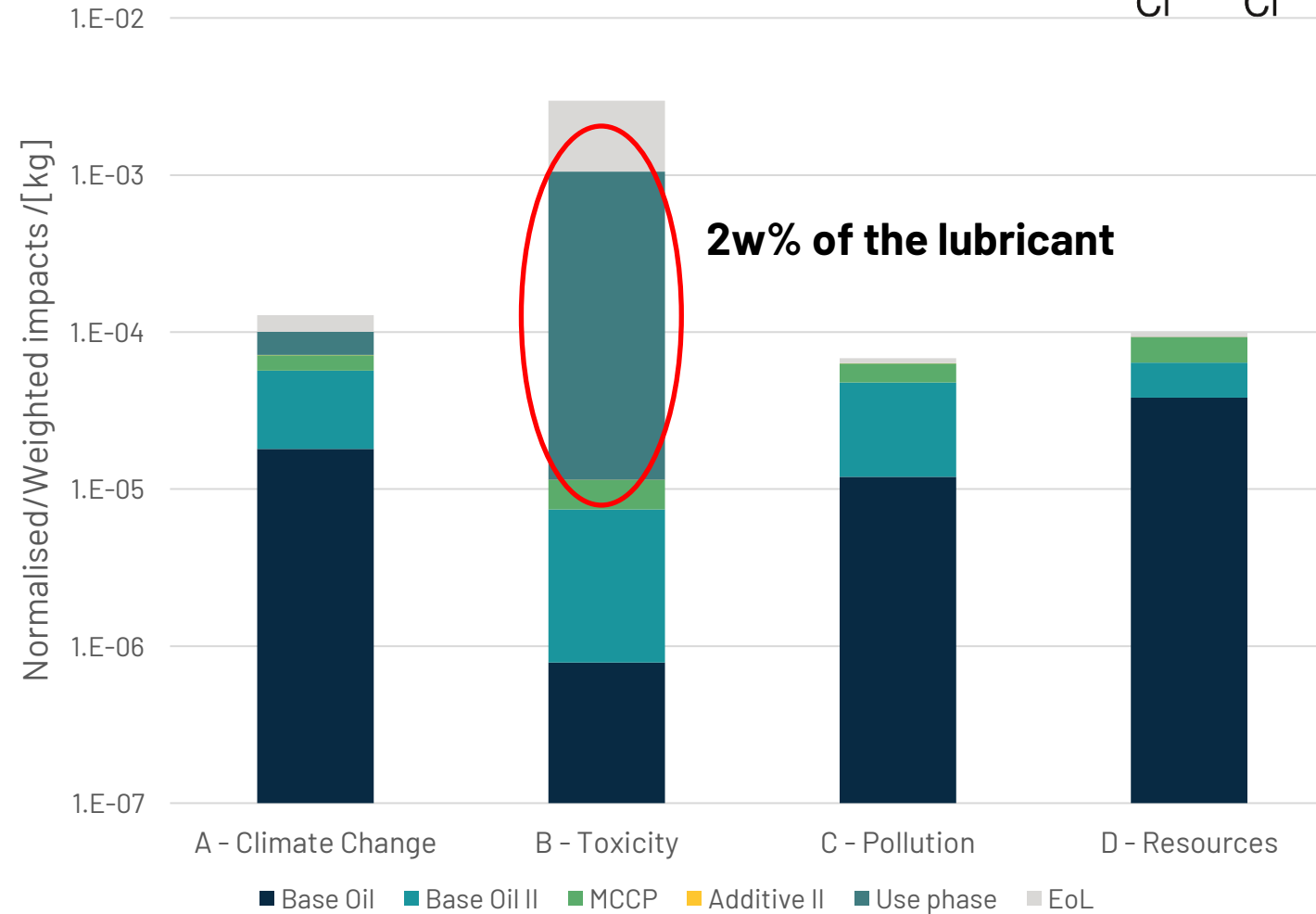


How does this translates to impacts?

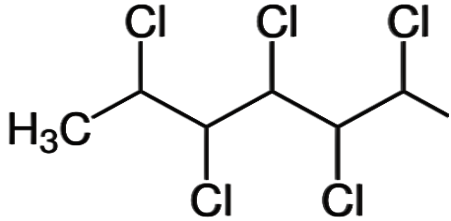
Results for MCCP formulation



- Results are obtained using ecoinvent 3.12
- LCIA with EF 3.1
- CFs for direct emission EF 3.1
- Normalization and weighting optimized for SSbD: A, B, C, D



But if we benchmark against a competitive formulation (sulfur-based with ester)?

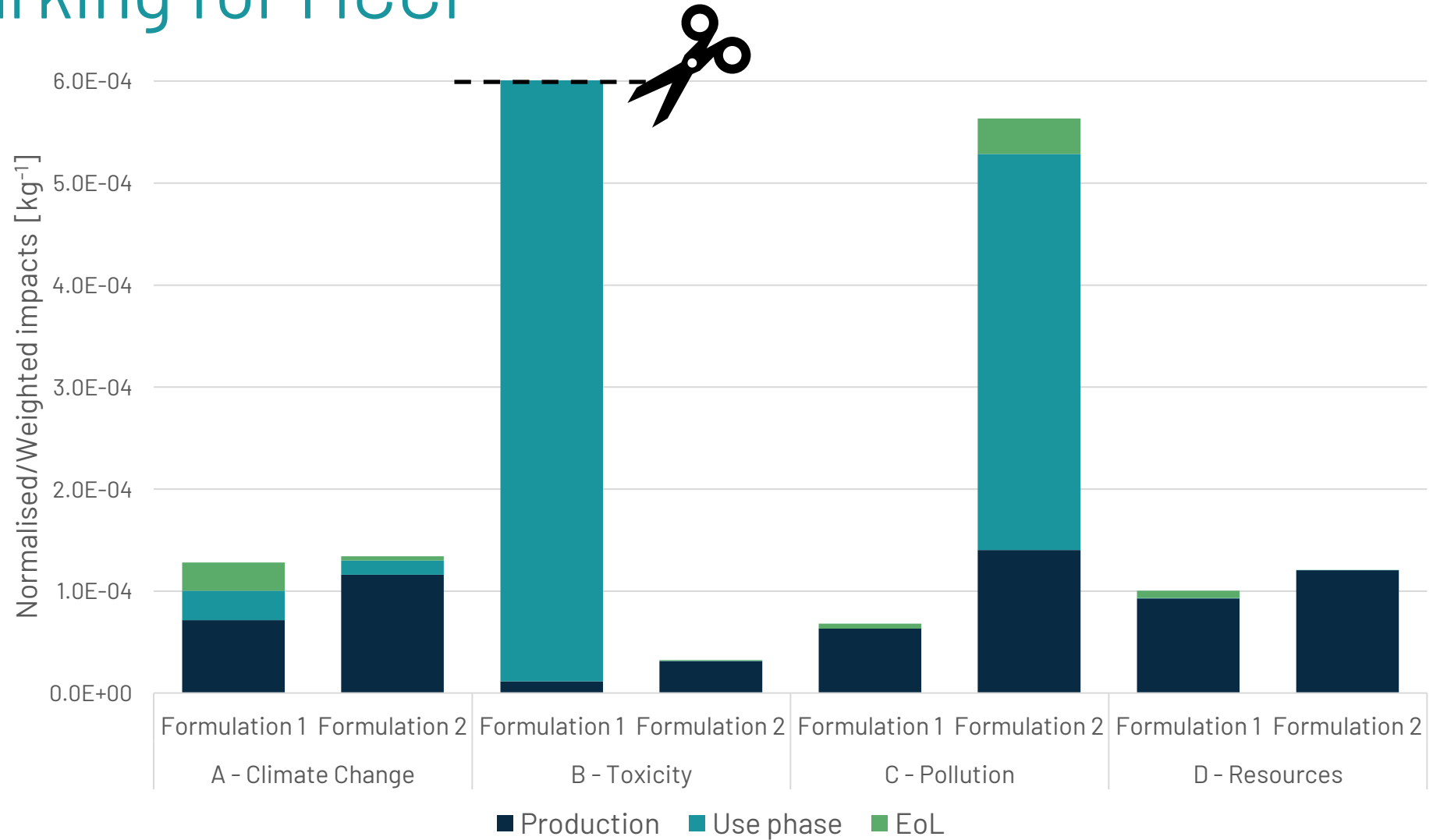


- **base oil (fossil)**
- **base oil (bio-based)**
- **~30w% MCCP**

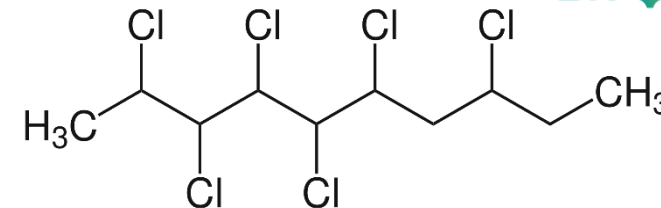
16 S 32.07

- **base oil (bio-based)**
- **~ 50w% sulfurized addit.**

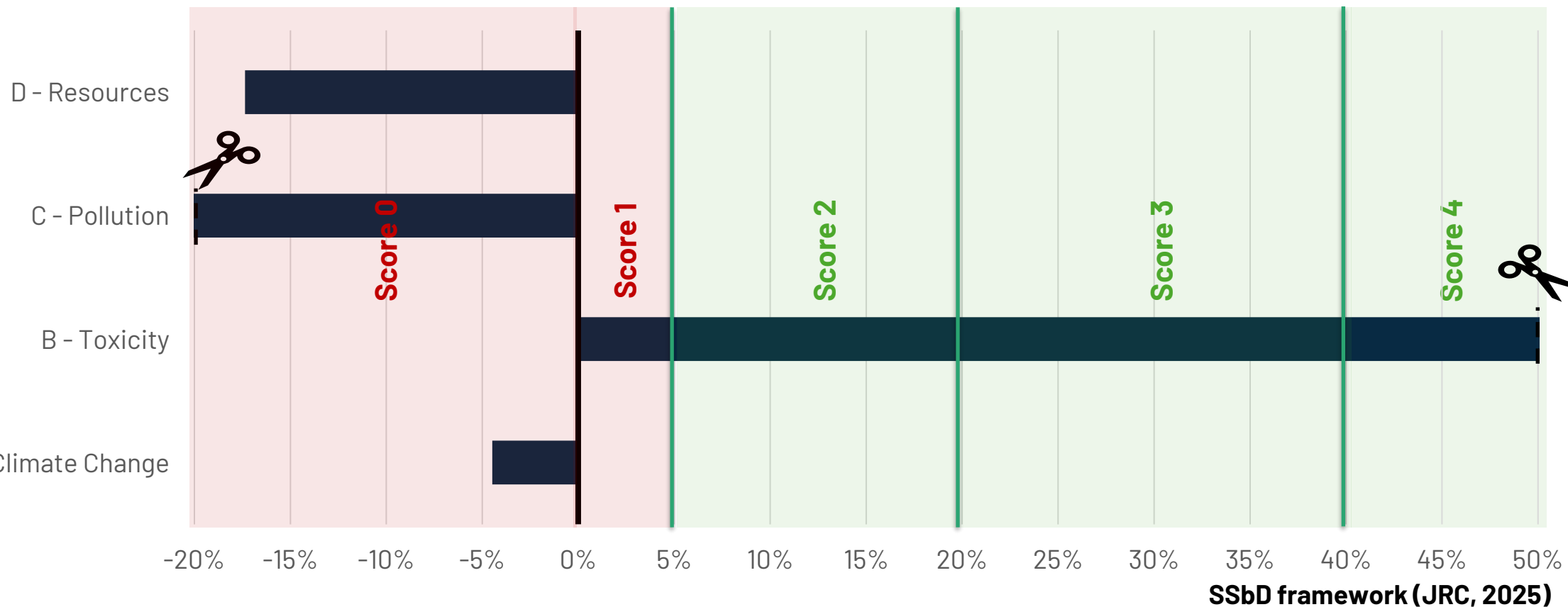
which is bio-based



Less toxic but more polluting (S→SO₂)

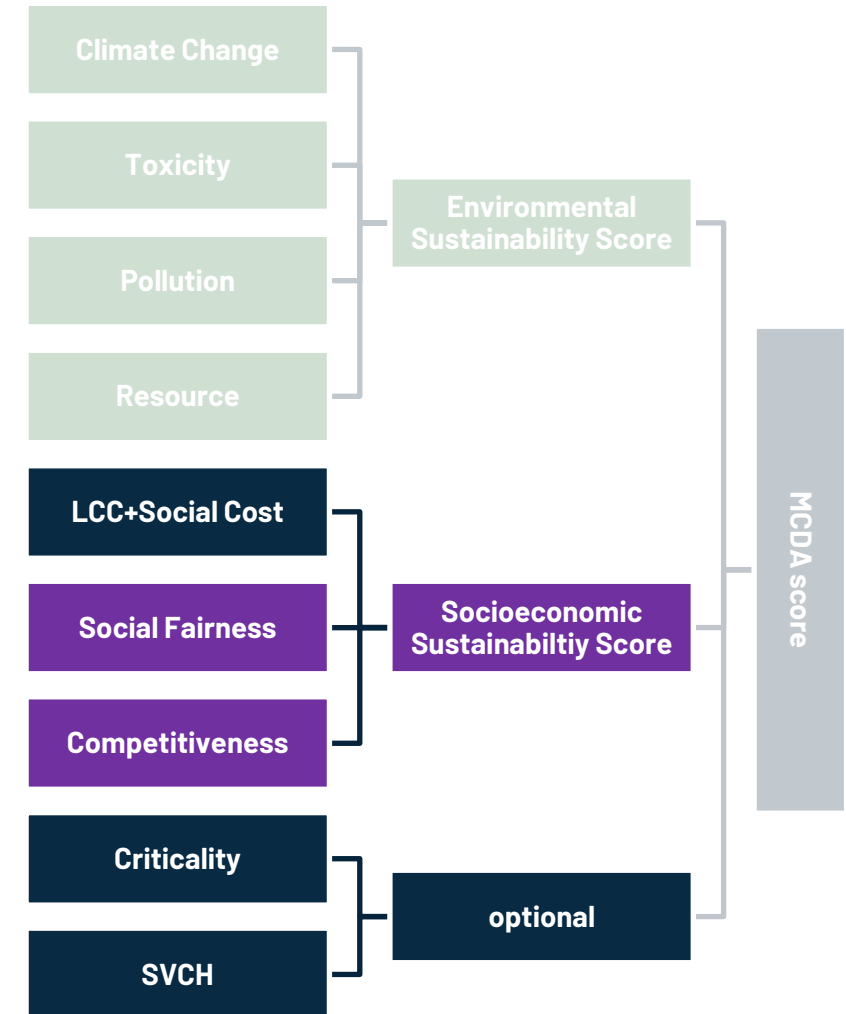
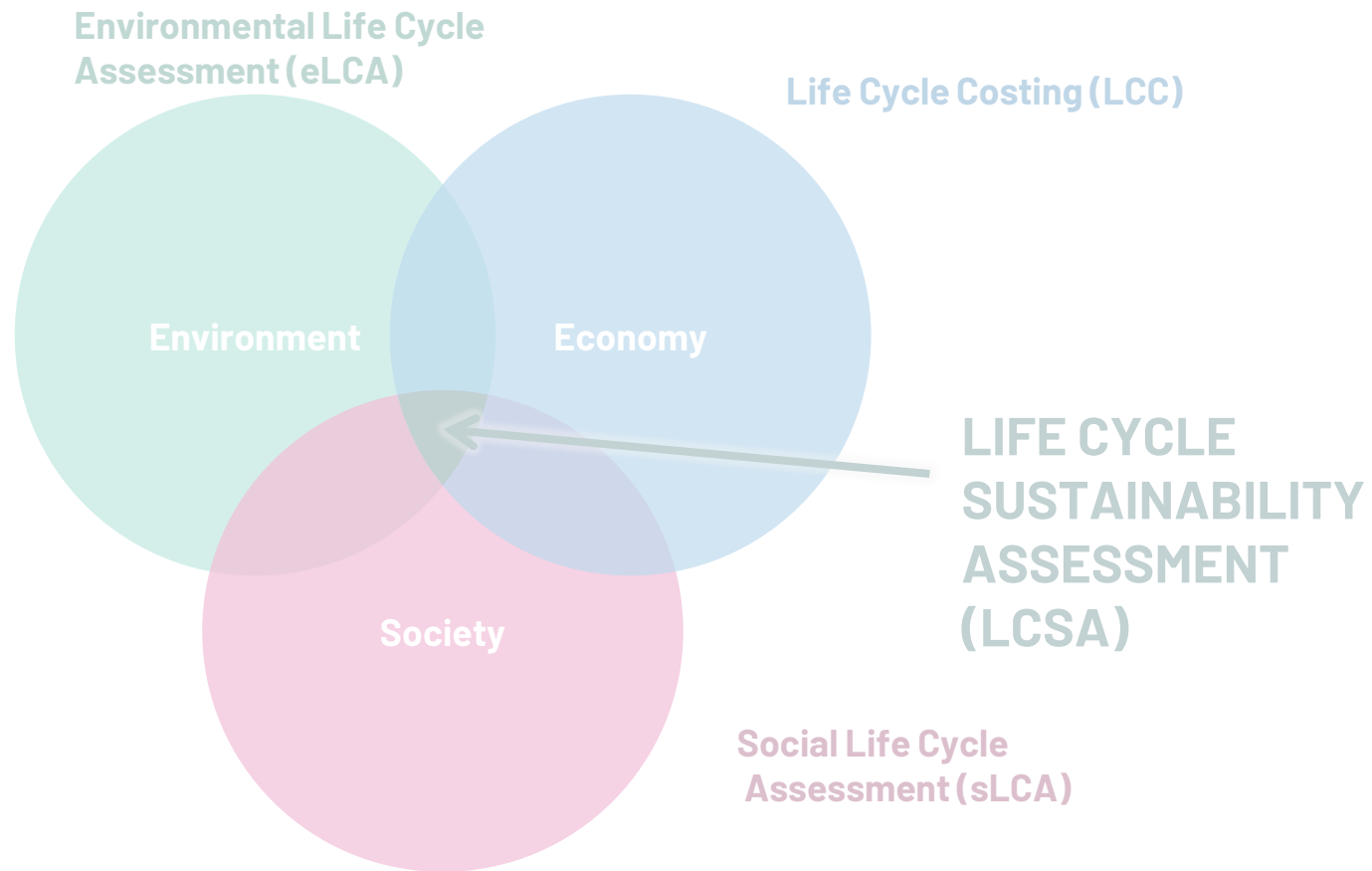


SSbD benchmarking (JRC values)



Besides Toxicity, the alternative is less environmental sustainable!

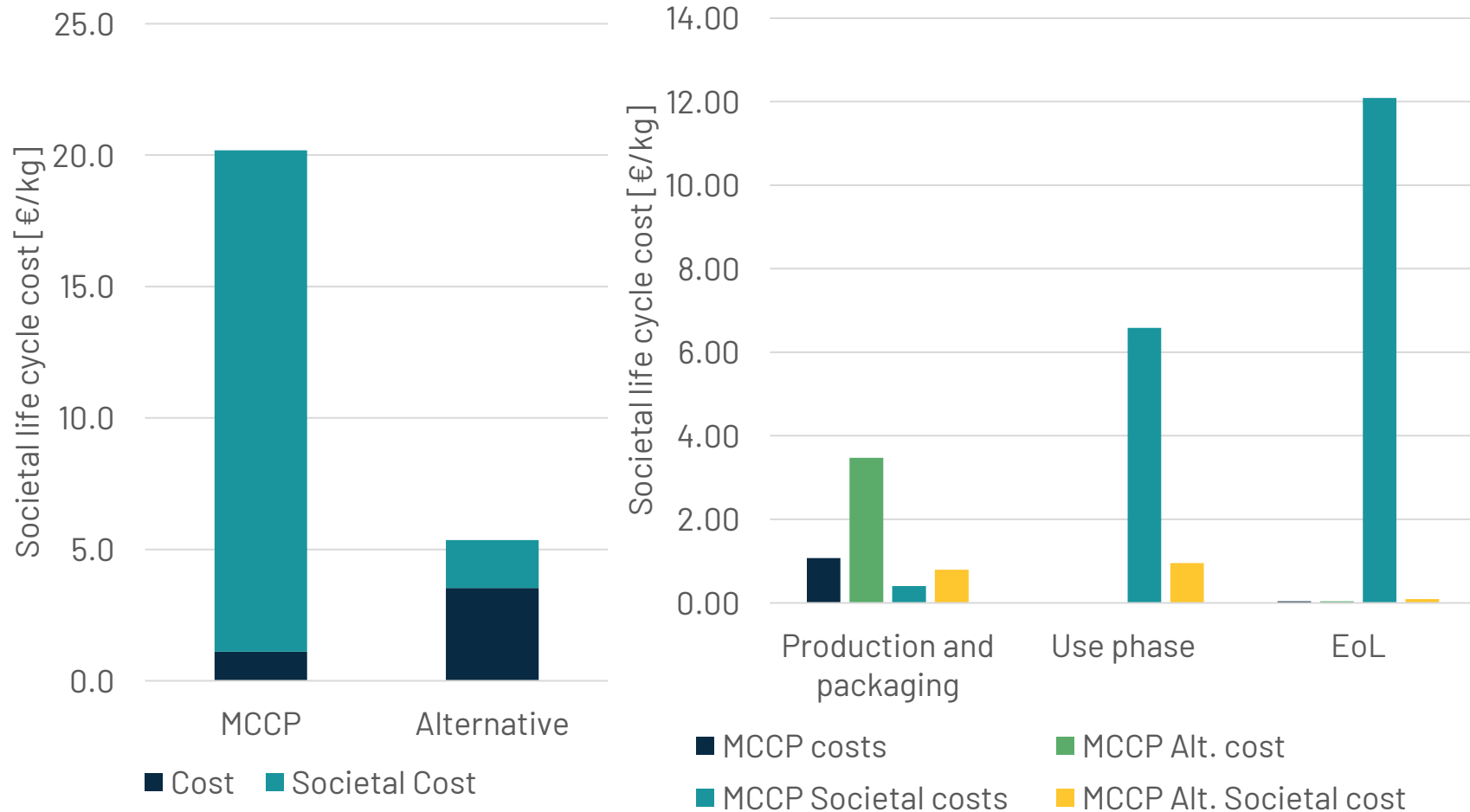
LCSA and SSbD – it is a match





Societal Life Cycle Costing vs. Alternative

- **Same inventory** as eLCA
- **Internal costs** from market data, own protocol and industry partners
- **External costs:** EF 3.1 results monetised with environmental prices (Gama Caldas et al., 2024) as in revised SSbD framework (JRC, 2025)

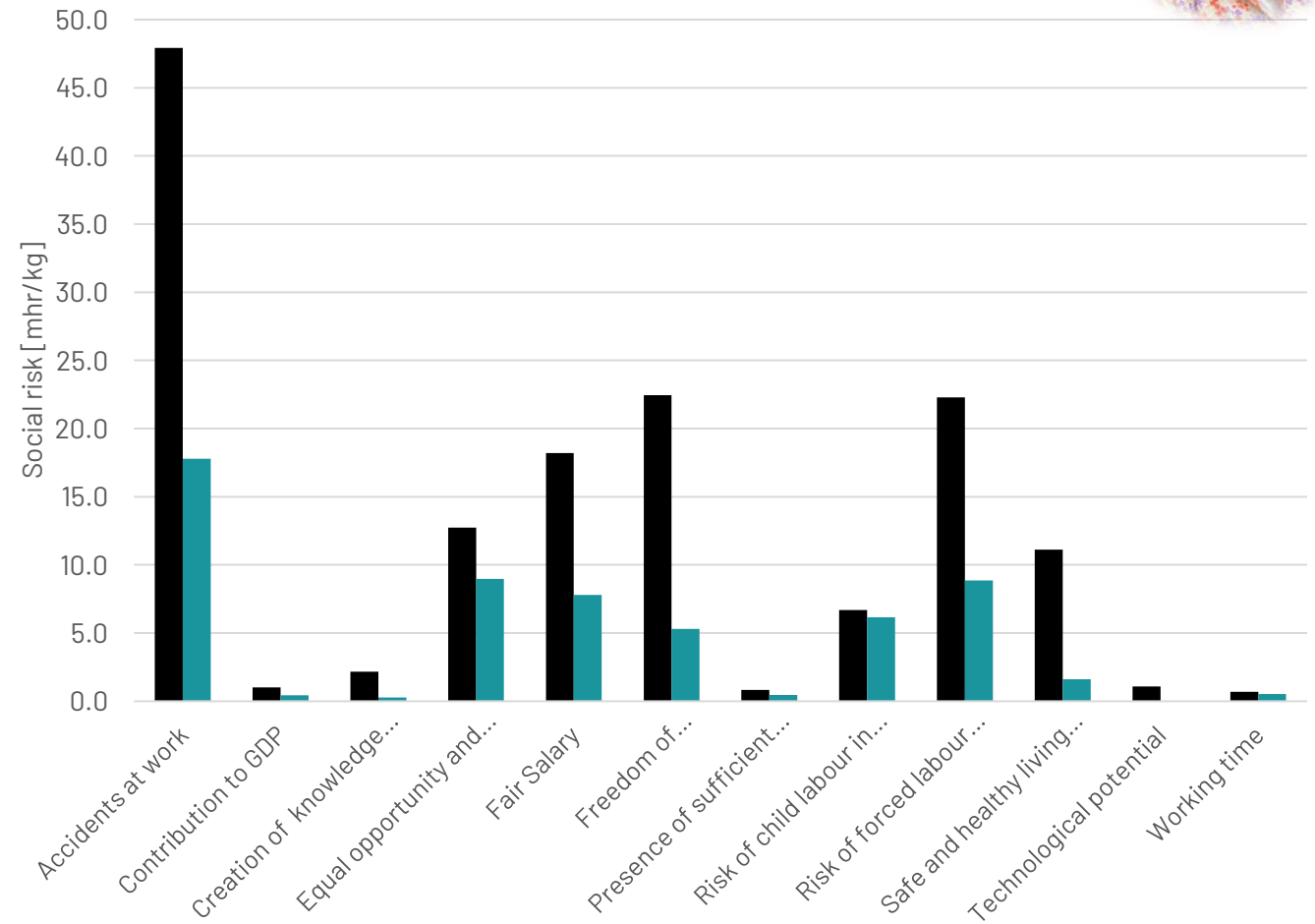
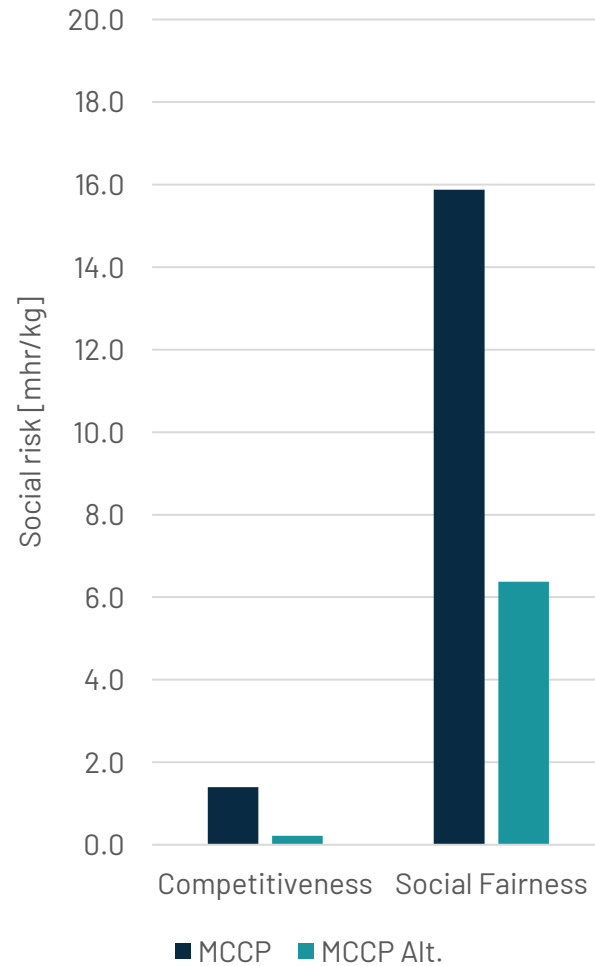


Total cost higher for the MCCP formulation besides more expensive!

Social LCA Results per pillar



- Same inventory as eLCA, linked to social risks via **soca v4** (Hamed & Ciroth, 2025)
- **Social indicators** selected according to the **SSbD framework** (JRC, 2025)
- Indicators grouped into **Competitiveness** and **Social Fairness**, weighted as in SiToLub



The bio-based alternative performs better socially overall by cutting petroleum- and chlorine-linked risks (Columbia) but holds own risk (e.g. child labour)

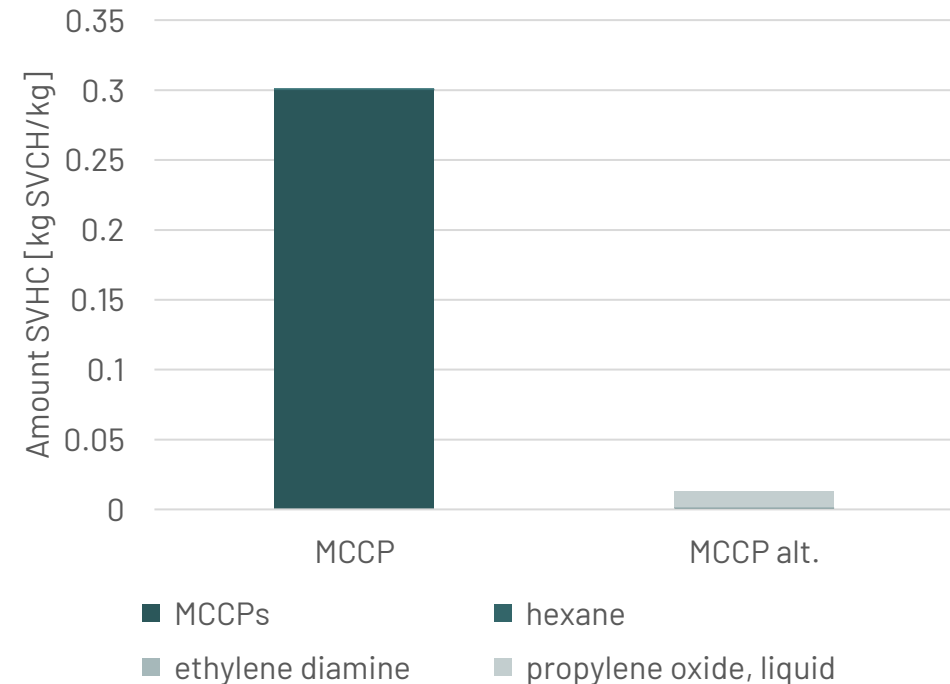
Criticality and SVCH Usage

- Critical Raw Material according to JRC CRM list
- Shadow flows tracked via ecoinvent process
- **Weighted** with SH2E factors (IR_i , SR_i , c_i ,

Name	Inventory res...	Characterization factor	Impact assessmen...
▼ SSbD CRM with SH2E CFs			4.30110E-10 dime...
> Phosphate Rock CRM	0.11999 kg	1.60000E-9 dimensionl...	1.91985E-10 di...
> Boron CRM	7.22267E-6 kg	1.92000E-5 dimensionl...	1.38675E-10 di...
> Lithium CRM	2.05083E-7 kg	0.00015 dimensionless/...	3.03850E-11 di...
> Magnesium CRM	9.19219E-5 kg	2.62000E-7 dimensionl...	2.40835E-11 di...
> Coking Coal CRM	0.28297 kg	6.87000E-11 dimension...	1.94403E-11 di...

Name	Inventory res...	Characterization factor	Impact assessment...
▼ SSbD CRM with SH2E CFs			1.34458E-10 dimen...
> Boron CRM	3.70535E-6 kg	1.92000E-5 dimension...	7.11426E-11 di...
> Phosphate Rock CRM	0.01119 kg	1.60000E-9 dimension...	1.78986E-11 di...
> Magnesium CRM	5.02537E-5 kg	2.62000E-7 dimension...	1.31665E-11 di...
> Lithium CRM	8.19362E-8 kg	0.00015 dimensionles...	1.21396E-11 di...
> Coking Coal CRM	0.16987 kg	6.87000E-11 dimensio...	1.16703E-11 di...
> Manganese CRM	0.00012 kg	3.51000E-8 dimension...	4.16665E-12 di...

- Added SVHCs from the **ECHA Candidate List** and added shadow flows at production
- **SVHC usage** adds to conduct detailed RA



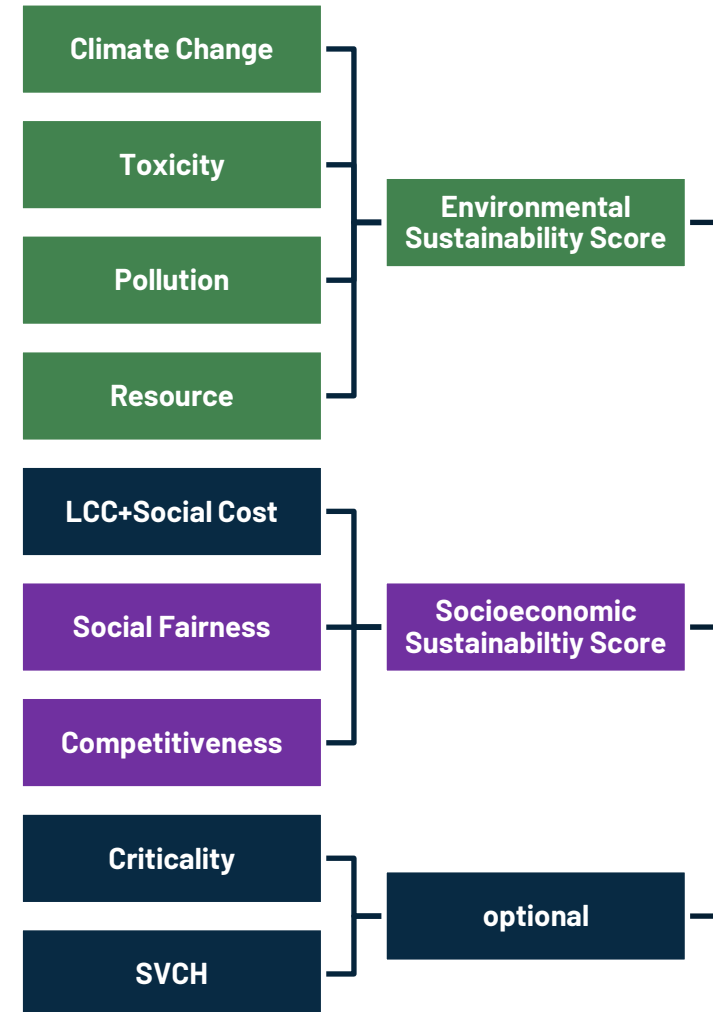
Criticality and SVCH Usage flagged from background adds value!

Conclusion and what is next?

- **The SiToLub model predicts the LCSA of four use cases with the full life cycle**
 - Follows the **SSbD approach** and design criteria, enabling **early screening**
 - **Automated production model** with **application-dependent** use phase and EoL
 - Toxicity in the foreground carries **USEtox uncertainty** in benchmarking → **log**
 - **eLCA does not favour the alternative**: oleate ester production is intensive
 - **Societal LCC favours** the safer and more sustainable alternative
 - **sLCA captures trade-offs** and social risks between alternatives
- **SVHC and CRM are valuable indicators that flag regulatory and supply risks**
- **The results have been presented to industrial stakeholders with great interest**

Next steps:

- **Variable, performance-based functional units (from DU to FU)**
- **Uncertainty framework across modelling approaches (retrosynthesis, stoichiometric, literature)**



**White paper on
weighting approaches
For LCSA in SSbD**



Thank you!

Jonas Hoffmann
GreenDelta GmbH
hoffmann@greendelta.com

**retroLCA
github repo**

