SITOLUB

SIMULATION TOOLS FOR THE DESIGN OF SAFE AND SUSTAINABLE LUBRICANTS

Integrated Simulation Approaches for Environmental and Socioeconomic Sustainability of SSbD-Compliant Lubricants

5th Stakeholder workshop on "Safe and sustainable by design"

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GreenDelta openLCA

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THE 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 and materials

Total cost: 6.23 Mio. €, 2024-2028
12 partners
5 EU countries
2 Associated countries

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SSbD CASES

INDUSTRY NEEDS

a) low friction **perfluoroalkyl substances** (persistent)

b) substitution of **chlorinated paraffins** (dioxins)

c) substitution of **corrosion inhibitors** (endocrine disruptor)

REACH COMPLIANT · COMPLIANT · COMPLIANT

EU Ecolabel www.ecolabel.eu

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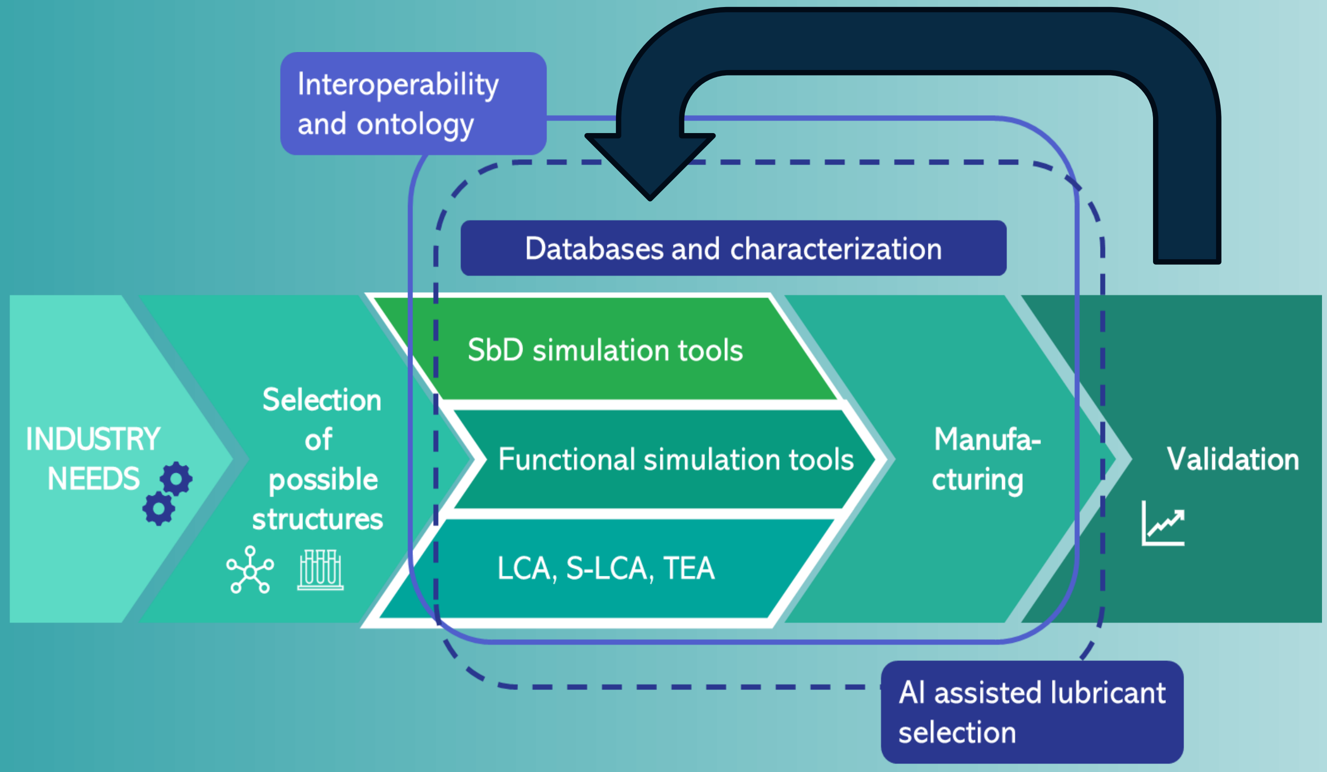
SITOLUB WORKING PLAN



Simulation of SSbD can be:

- **Cheaper**
- **Faster**

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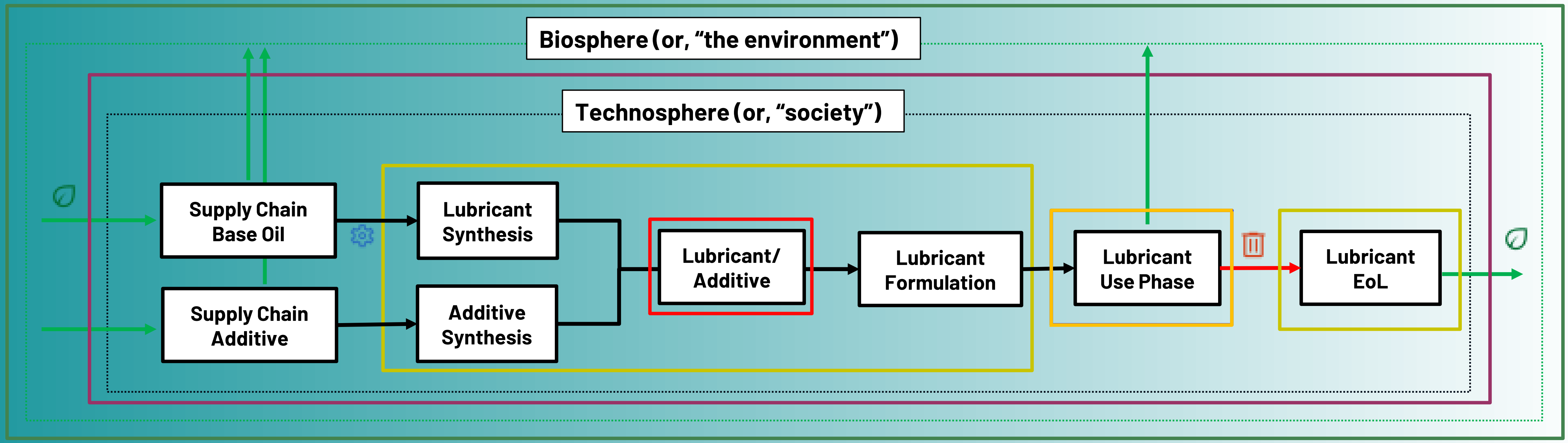
SITOLUB SSbD FRAMEWORK



SAFETY: Hazard Assessment | Risk Assessment during Processing | Risk Assessment in Application

SUSTAINABILITY: Performance Assessment | Environmental Impact Assessment | Socio-economic Assessment

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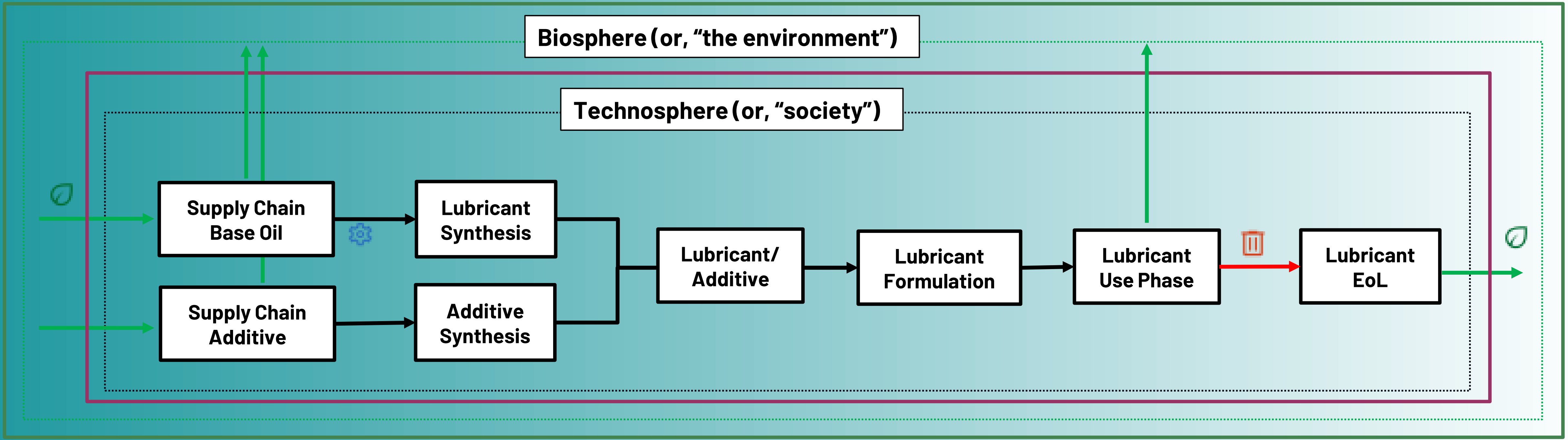
SITOLUB SSbD FRAMEWORK



SAFETY:

SUSTAINABILITY: GreenDelta

Environmental Impact Assessment | Socio-economic Assessment

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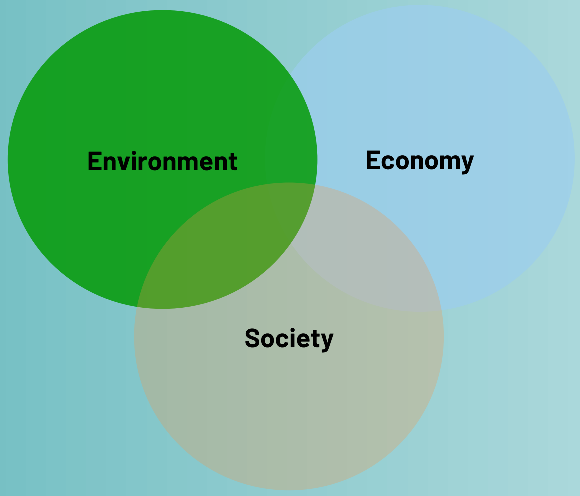
Step 4: Environmental Sustainability Assessment



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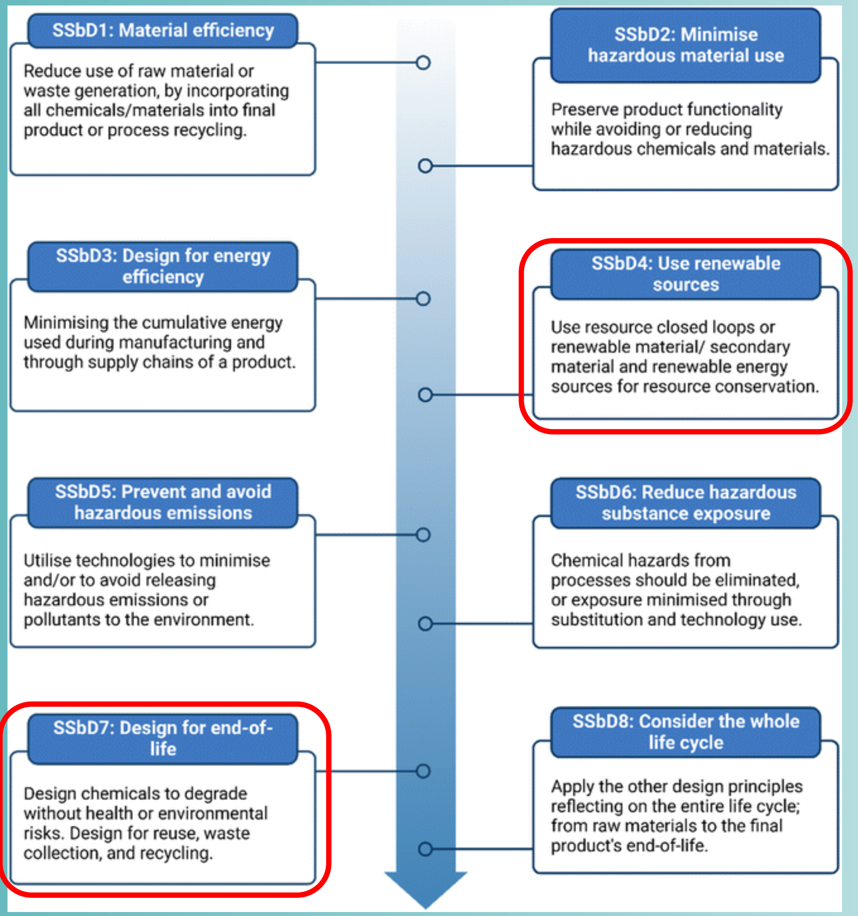
SSbD-COMPLIANT LUBRICANTS

Petrol-based lubricants



Bio-based lubricants

Lennon et al., **RSC Sustain.**, 2024,2, 578-607

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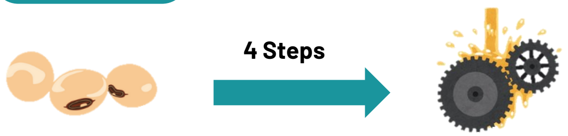
PRODUCTION: BIO VS. PETROL-BASED LUBRICANT

Our model



Refined soybean-oil

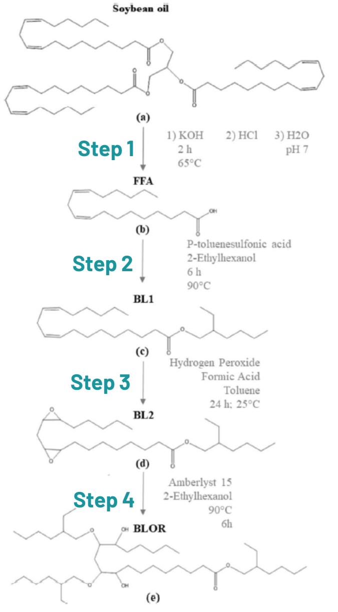
High performance Bio-based lubricant

Step 1: Hydrolysis

Step 2: Esterification

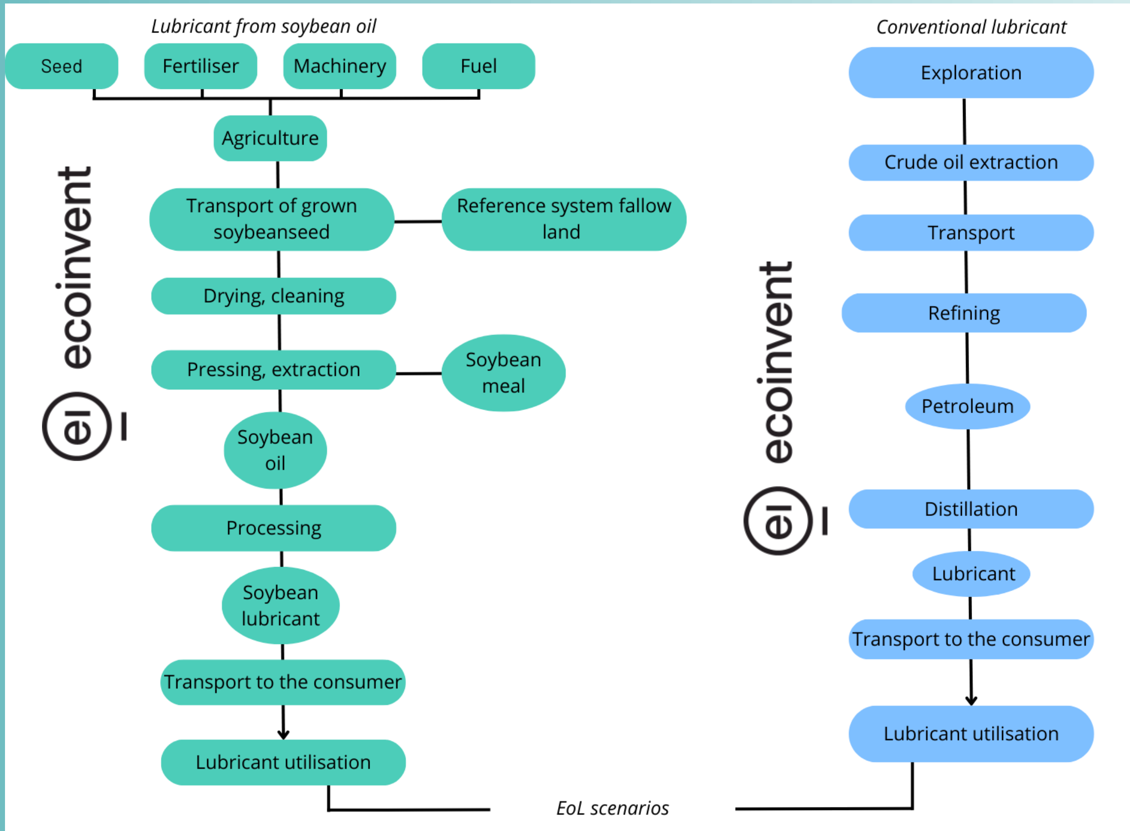
Step 3: Epoxidation

Step 4: Ring opening



de Luna et al. *Biomass Conv. Bioref* **2023**, DOI 10.1007/s13399-023-04395-3.

Production process



Comparative life cycle assessment of biolubricants and mineral based lubricants, Cuevas, ***2005***

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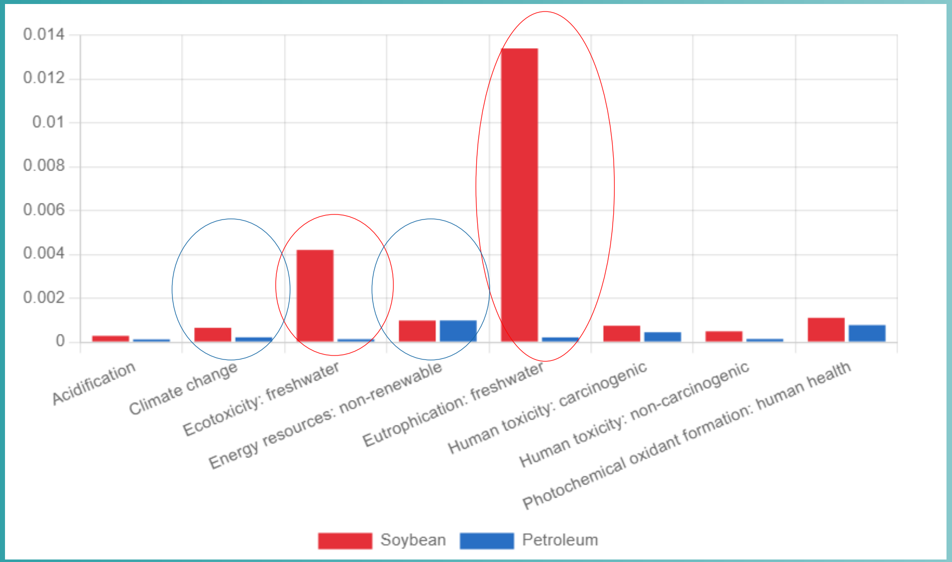
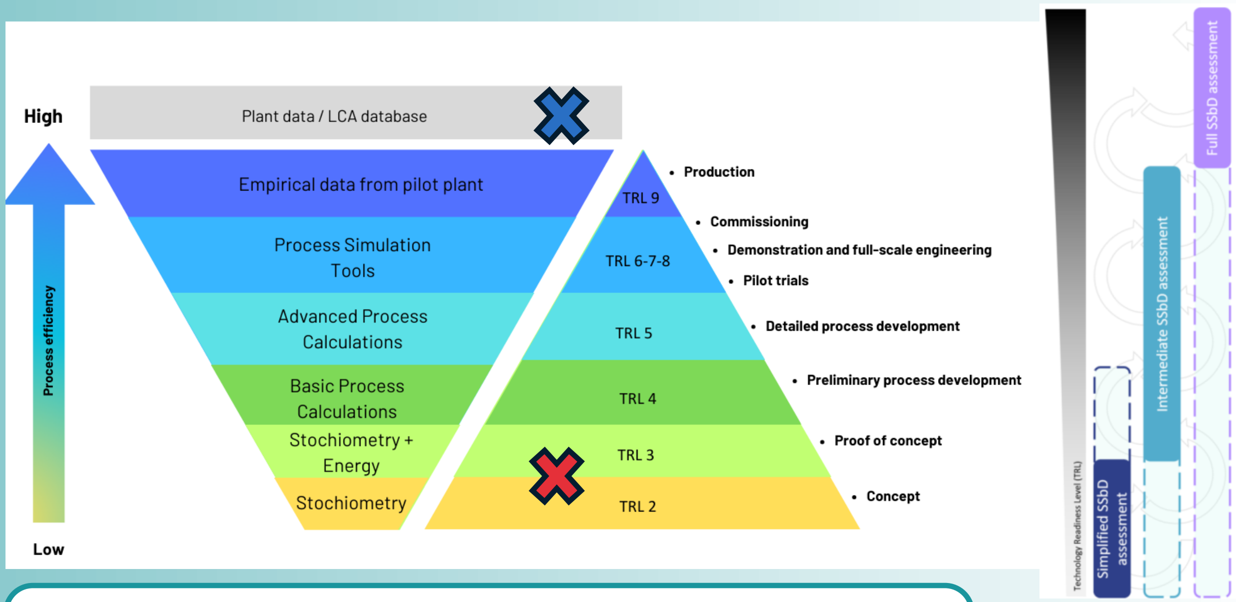
LCIA: BIO VS. PETROL-BASED LUBRICANT

Normalized bar chart, referenced to 1 kg, ecoinvent 3.10 cut-off, EF 3.1 method





→Eutrophication and Ecotoxicity are up ✓
→Fossil use and climate change as well ✗

→Mismatching model approach (stochiom., no scale up) and TRL level result in biased data!

→Novel bio-lubricant would not be 'more sustainable' than existing technologies?

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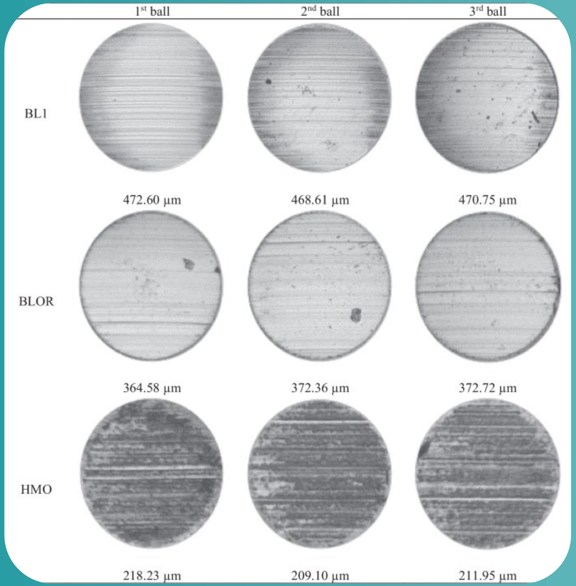
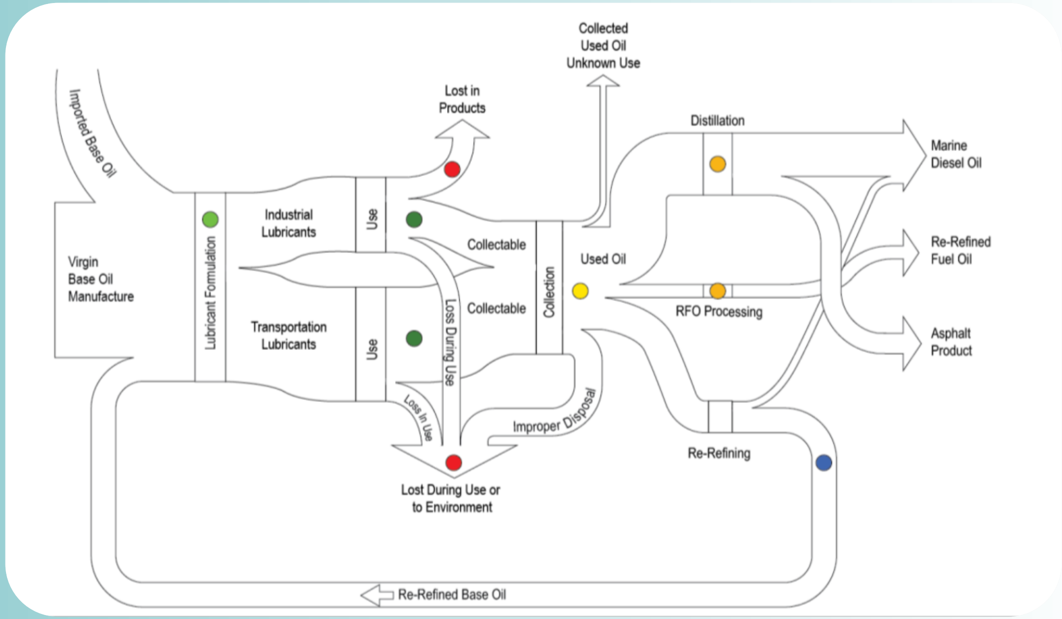
USE PHASE AND EoL



de Luna et al. *Biomass Conv. Bioref* **2023**

Products	Functional unit
Mineral oil Rapeseed oil	1 kg of oil
Mineral oil Synthetic ester Rapeseed oil	1 m^3 of hydraulic fluid
Mineral oil Soybean oil	Area of aluminium rolled
Mineral oil Rapeseed oil ester Palm oil ester Animal fat ester Used cooking oil ester	1000 work pieces produced
Mineral oil Rapeseed oil	Volume of oil used to cut 1000 m^3 of wood[b]

Cavallaro et al. *Environmental life-cycle assessment (LCA) of lubricants* **2013** *Biolubricants*, 527–564.



Used Oil Management and Beneficial Reuse Options to Address Section 1: Energy Savings from Lubricating Oil Public Law 115-345, Report to Congress, **2020**, Washing.

Wear protection

Performance-based FU

Various EoL options

SSbD7: Design for end-of-life

Design chemicals to degrade without health or environmental risks. Design for reuse, waste collection, and recycling.

→ We need to further integrate 'sustainable performance' at low TRL

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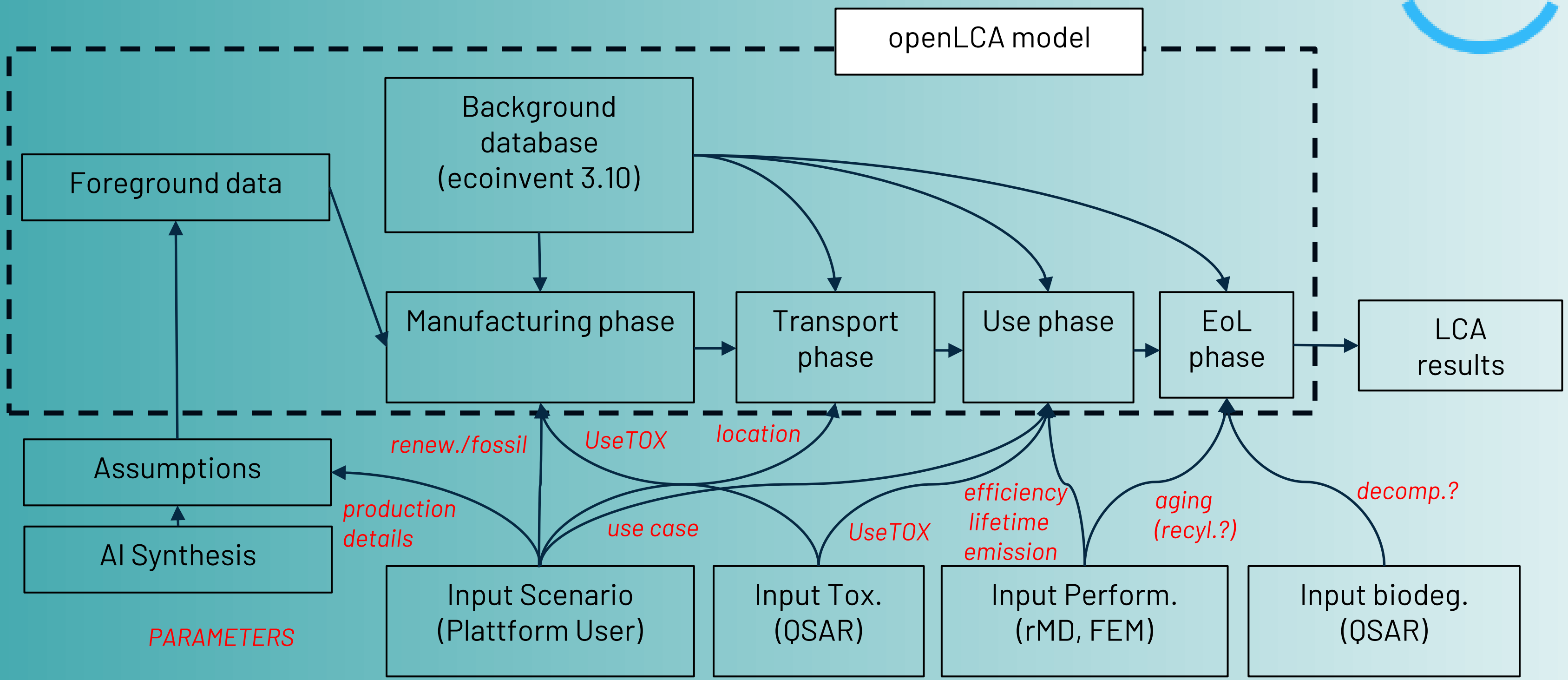
FULL LIFE CYCLE WITH PARAMETERS



→ Parametrized LCAs will allow fully integrated SSbD approaches

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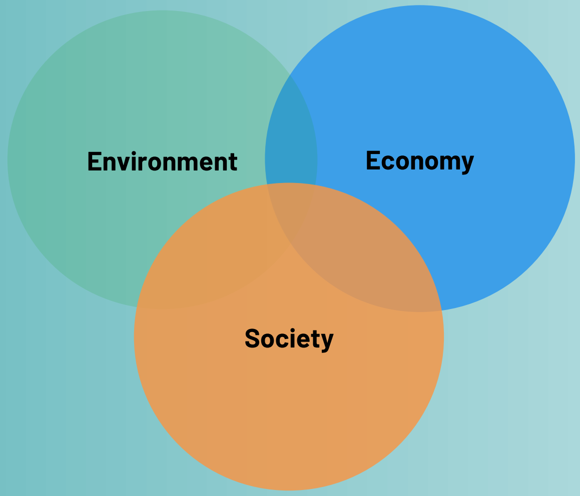
(Step 5:) Socio-economic assessment



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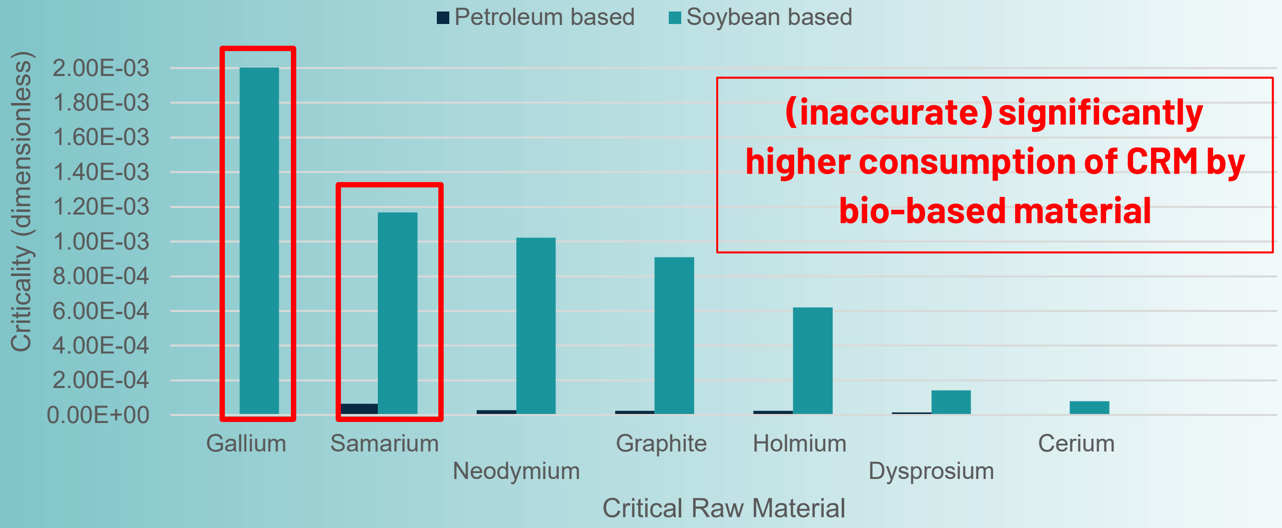
CRITICALITY ASSESSMENT

Following the logic of LCA, Bargiacchi et al. (2022) and Zapp and Schreiber (2021) proposed a **criticality indicator** where characterization factors (CF) can be calculated by:

$$CF = \frac{SR_i}{c_i \cdot \left(1 - IR_i \cdot \left(1 - EoL_{RIR}\right)\right)}$$

SR_i Supply Risk of resource i
c_i European consumption of resource i
IR_i Import reliance of resource i
EoL_{RIR} End-of-life recycling input rate

Comparison between two lubricants using generic information



- Link to ecoinvent database to be able to **calculate the CRM** on both the supply chain and the foreground data
- **Limitations** of relying on generic databases **for low TRL**
- Supply chain for soybean could be linked to **incorrect industries**

Bargiacchi E, Puig-Samper G, Campos-Carriedo F, Iribarren D, Dufour J, Ciroth A, et al. D2.2 Definition of FCH-LCA guidelines WP2 Reformulation of current guidelines for Life Cycle Assessment. 2022. Zapp P, Schreiber A. D3.1 Material criticality indicator. Brussels: Clean Hydrogen Partnership; 2021

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Social LCA – Preliminary comparative assessment

soca = ecoinvent + PSILCA

Petro-based lubricant - created

Indicator results

	HO	MO	LO	NOP	NOR	VLR	LR	MR	HR	VHR	ND	NA
Local Community	0%	0%	0%	0%	10%	15%	16%	17%	16%	10%	16%	0%
Access to material resources	0%	0%	0%	0%	0%	58%	9%	11%	6%	16%	1%	0%
Environmental Footprints	0%	0%	0%	0%	49%	6%	17%	14%	1%	12%	1%	0%
GHG Footprints	0%	0%	0%	0%	4%	0%	0%	49%	47%	0%	0%	0%
Local employment	0%	0%	0%	0%	0%	0%	39%	2%	1%	7%	51%	0%
Migration	0%	0%	0%	0%	0%	20%	8%	8%	7%	1%	56%	0%
Respect of indigenous rights	0%	0%	0%	0%	20%	0%	27%	31%	18%	0%	3%	0%
Safe and healthy living conditions	0%	0%	0%	0%	0%	17%	15%	3%	30%	35%	0%	0%
Society	1%	2%	3%	0%	1%	38%	10%	9%	25%	11%	0%	0%
Contribution to economic development	2%	4%	5%	0%	0%	39%	8%	6%	22%	14%	0%	0%
Health and Safety	0%	0%	0%	0%	1%	38%	11%	12%	29%	8%	0%	0%
Value Chain Actors	0%	0%	0%	0%	0%	3%	9%	29%	12%	29%	17%	0%
Corruption	0%	0%	0%	0%	0%	6%	4%	34%	1%	32%	24%	0%
Fair competition	0%	0%	0%	0%	0%	3%	24%	0%	5%	48%	19%	0%
Promoting social responsibilty	0%	0%	0%	0%	0%	0%	0%	54%	31%	8%	7%	0%
Workers	0%	0%	0%	0%	5%	25%	22%	16%	8%	10%	12%	0%
Child labour	0%	0%	0%	0%	1%	85%	14%	0%	0%	0%	0%	0%
Discrimination	0%	0%	0%	0%	0%	39%	2%	23%	4%	4%	28%	0%
Fair Salary	0%	0%	0%	0%	0%	18%	30%	20%	2%	30%	0%	0%
Forced Labour	0%	0%	0%	0%	0%	18%	30%	16%	2%	1%	33%	0%
Freedom of association and collective bargaining	0%	0%	0%	0%	41%	0%	29%	0%	3%	22%	5%	0%
Health and Safety	0%	0%	0%	0%	0%	35%	16%	13%	0%	6%	30%	0%
Social benefits, legal issues	0%	0%	0%	0%	0%	6%	13%	51%	9%	21%	0%	0%
Working time	0%	0%	0%	0%	0%	0%	47%	7%	47%	0%	0%	0%

Soybean lubricant

Indicator results

	HO	MO	LO	NOP	NOR	VLR	LR	MR	HR	VHR	ND	NA
Local Community	0%	0%	0%	0%	8%	17%	17%	18%	12%	10%	17%	0%
Access to material resources	0%	0%	0%	0%	0%	54%	20%	8%	3%	12%	1%	0%
Environmental Footprints	0%	0%	0%	0%	44%	7%	27%	8%	3%	10%	1%	0%
GHG Footprints	0%	0%	0%	0%	5%	0%	0%	52%	43%	0%	0%	0%
Local employment	0%	0%	0%	0%	0%	0%	18%	4%	2%	8%	68%	0%
Migration	0%	0%	0%	0%	0%	30%	8%	8%	5%	3%	46%	0%
Respect of indigenous rights	0%	0%	0%	0%	10%	1%	33%	43%	9%	0%	4%	0%
Safe and healthy living conditions	0%	0%	0%	0%	0%	24%	16%	4%	20%	34%	1%	0%
Society	1%	1%	4%	0%	3%	33%	18%	13%	19%	9%	0%	0%
Contribution to economic development	2%	2%	7%	0%	0%	31%	18%	13%	16%	12%	0%	0%
Health and Safety	0%	0%	0%	0%	6%	34%	17%	14%	22%	7%	0%	0%
Value Chain Actors	0%	0%	0%	0%	0%	3%	6%	23%	12%	37%	19%	0%
Corruption	0%	0%	0%	0%	0%	6%	17%	21%	2%	34%	21%	0%
Fair competition	0%	0%	0%	0%	0%	4%	1%	0%	24%	47%	23%	0%
Promoting social responsibilty	0%	0%	0%	0%	0%	0%	0%	47%	11%	31%	11%	0%
Workers	0%	0%	0%	0%	6%	26%	18%	16%	12%	9%	12%	0%
Child labour	0%	0%	0%	0%	2%	82%	15%	0%	0%	0%	0%	0%
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Forced Labour	0%	0%	0%	0%	0%	20%	28%	15%	3%	1%	33%	0%
Freedom of association and collective bargaining	0%	0%	0%	0%	48%	0%	18%	0%	5%	20%	9%	0%
Health and Safety	0%	0%	0%	0%	0%	41%	15%	9%	1%	3%	33%	0%
Social benefits, legal issues	0%	0%	0%	0%	0%	7%	3%	55%	19%	16%	0%	0%
Working time	0%	0%	0%	0%	0%	0%	27%	10%	62%	0%	0%	0%

HO/MO/LO High/Medium/Low Opportunity, VLR/LR/MR/HR/VHR Very Low Risk, Low Risk, Medium Risk, High Risk, Very High Risk, ND No Data, NA Not Available

- Based on the **LCA database** and **LCC data**, the **sLCA** can be performed in **one database** (SOCA)
- **Petrol-based lubricant** shows **higher risks** for stakeholders "**workers**", "**local community**", and "**society**"
  - Indicators: "**Safe and healthy living conditions**" and "**Health and Safety**"

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sLCA- SELECTION ON SOCIAL INDICATORS

- **Selection** of the **indicators for SSbD** remains **challenging**
- While performing materiality assessment is needed as it depends on the stakeholders involved in the study – can be used as a complementary assessment
- However, **stakeholders/expert judgement** should not only be the contributing to the decision making but also **policy/action plan goals and literature surveying**
- Therefore, it **is recommended to establish a set of indicators** that is **mandatory** to assess in each life cycle

Social topics	1. Raw materials acquisition and pre-processing	2. Manufacturing	3. Distribution	4. Use	5. End of life
1. Access to material resources	5	5	3	1	1
2. Affordability	3	4	2	4	1
3. Child labour	5	5	1	1	1
4. Community engagement	4	3	1	1	1
5. Contribution to economic development	5	3	3	3	1
6. Corruption	5	5	4	3	1
7. Delocalization and migration	4	4	1	1	1
8. Discrimination and equal opportunities	4	4	1	1	1
9. Health and safety	5	5	5	1	1

Abbate, E., Garmendia Aguirre, I., Bracalente, G., Mancini, L., Tosches, D., Rasmussen, K., Bennett, M.J., Rauscher, H. and Sala, S., Safe and Sustainable by Design chemicals and materials - Methodological Guidance, Publications Office of the European Union, Luxembourg, 2024, doi:10.2760/28450, JRC138035.

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Conclusion:

Instead of **empirical** SSbD studies, **SiToLub** focuses on **simulation!**

In LCA data/methods, there is a **strong bias** on **existing technologies**

For functional materials assess **full life cycle (Use Cases, EoL options, Performance) already at early stage!**

Social Sustainability

Selecting social indicators requires **harmonization**

→ We argue for data-driven, integrated SSbD solutions allowing simulation

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