SITOLUB

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SIMULATION TOOLS FOR THE DESIGN OF SAFE AND SUSTAINABLE LUBRICANTS

Integrated SSbD Approach to Simulating the Sustainability of Lubricants: Challenges and Insights

GreenDeLTa

Dr. Jonas Hoffmann, Dr. Andreas Ciroth

openLca

SETAC, 35th, Vienna

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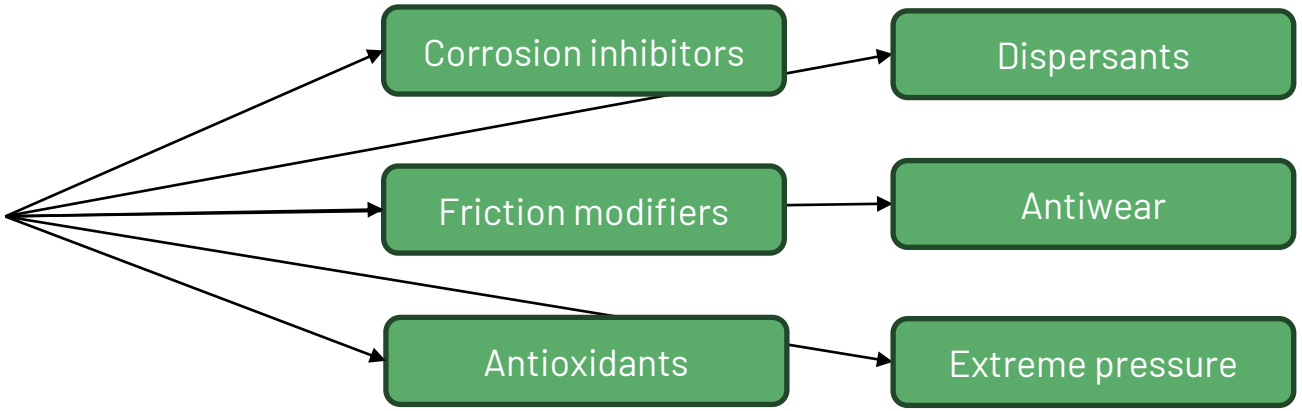
COMPONENTS OF LUBRICANTS

API BASE OIL CATEGORIES					
	Base Oil Category	Sulfur (%)		Saturates (%)	Viscosity Index
Mineral	Group I (solvent refined)	>0.03	and/or	<90	80 to 120
Mineral	Group II (hydrotreated)	<0.03	and	>90	80 to 120
Mineral	Group III (hydrocracked)	<0.03	and	>90	>120
Synthetic	Group IV	PAO Synthetic Lubricants			
Synthetic	Group V	All other base oils not included in Groups I, II, III or IV			



What industry is facing:

What costumers want:

REACH COMPLIANT · COMPLIANT · COMPLIANT

EU Ecolabel www.ecolabel.eu

BLAUER ENGEL DAS UMWELTZEICHEN

Industry is in need for novel safe and sustainable solutions!

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SSbD Framework – Fit For Purpose?

SSbD framework was tested with industry on:

A) Plasticizer

B) Flame retardants

C) Surfactants

Some outcome of the studies were (industry perspective):

- **Too complicated** exp. tests even for already known compounds
- **Too expensive** procedure and not fit for purpose

Industry is in need for SSbD simulation tools!

Caldeira, C., Garmendia Aguirre, I., Tosches, D., Mancini, L., Abbate, E., Farcal, R., Lipsa, D., Rasmussen, K., Rauscher, H., Riego Sintes, J. and Sala, S., Safe and Sustainable by Design chemicals and materials - Application of the SSbD framework to case studies, Publications Office of the European Union, Luxembourg, 2023, doi:10.2760/329423, JRC131878.

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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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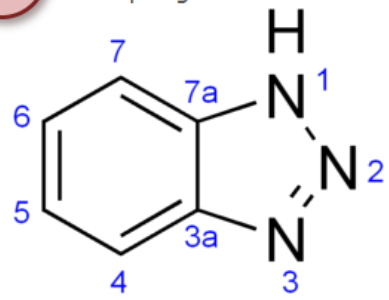
WORKING FLOW

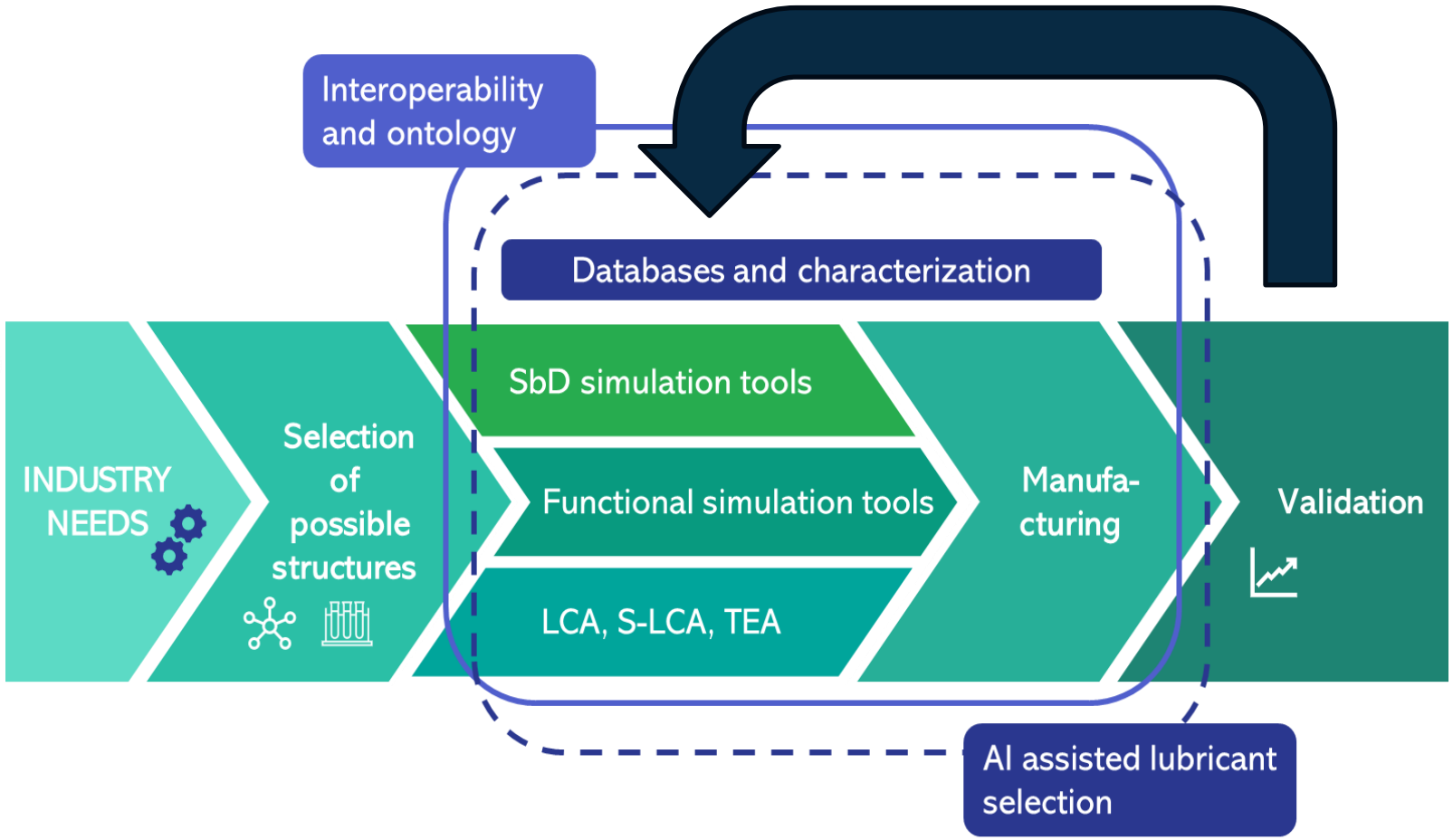
Properties of concern

PBT Under assessment as Persistent, Bioaccumulative and Toxic

ED Under assessment as Endocrine Disrupting



benzotriazole



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SITOLUB SIMULATION APPROACH

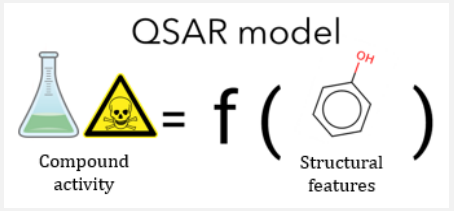
QSAR Simulation

Quantitative

Structural

Activity

Relationships

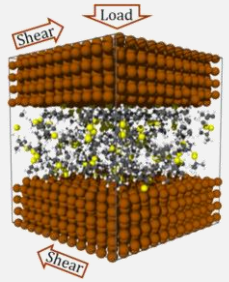


(Eco)Tox. & Biodegr.

Performance Sim.

- Evaluation for lubricants and their components

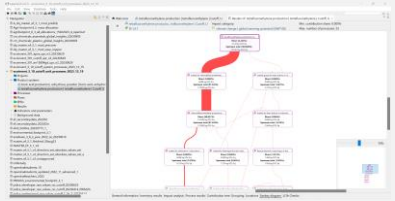
- Reactive MD simulation



Performance

Sustainability Sim.

- Environmental Impacts
- Social Impacts
- Economical Costs



Sustainability

AI-supported lubricant selection and data synthesis

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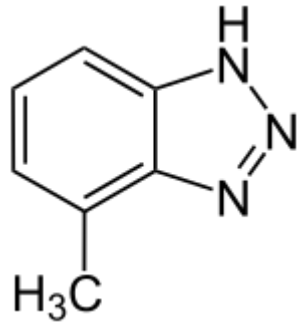
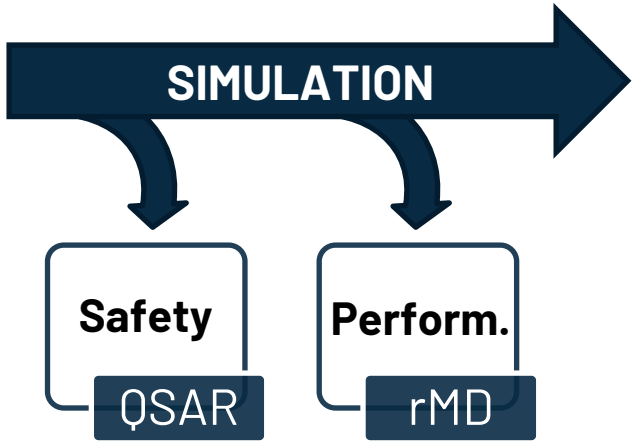
The Challenge:
Predict LCA for the entire life cycle

Platform – Input

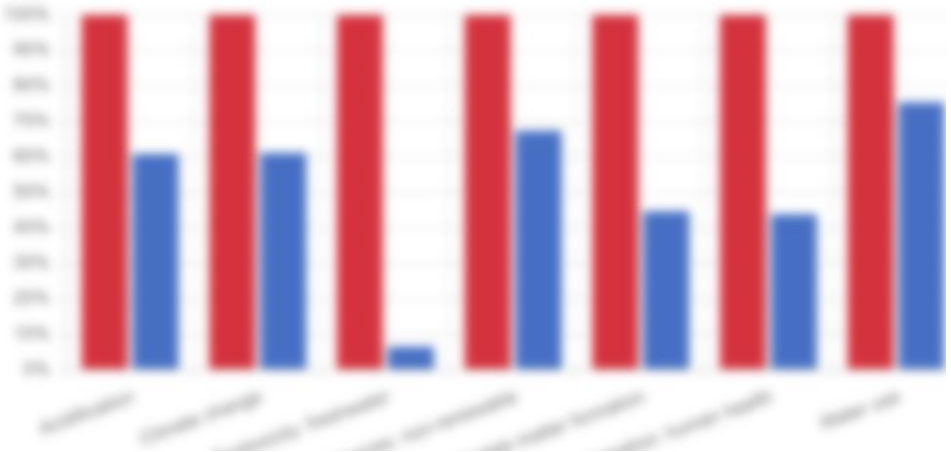


n1c2ccccc2[nH]n1

SMILES CODE
(or CAS)



Platform - Output



ENVIRONMENTAL IMPACTS
Cradle-to-Grave

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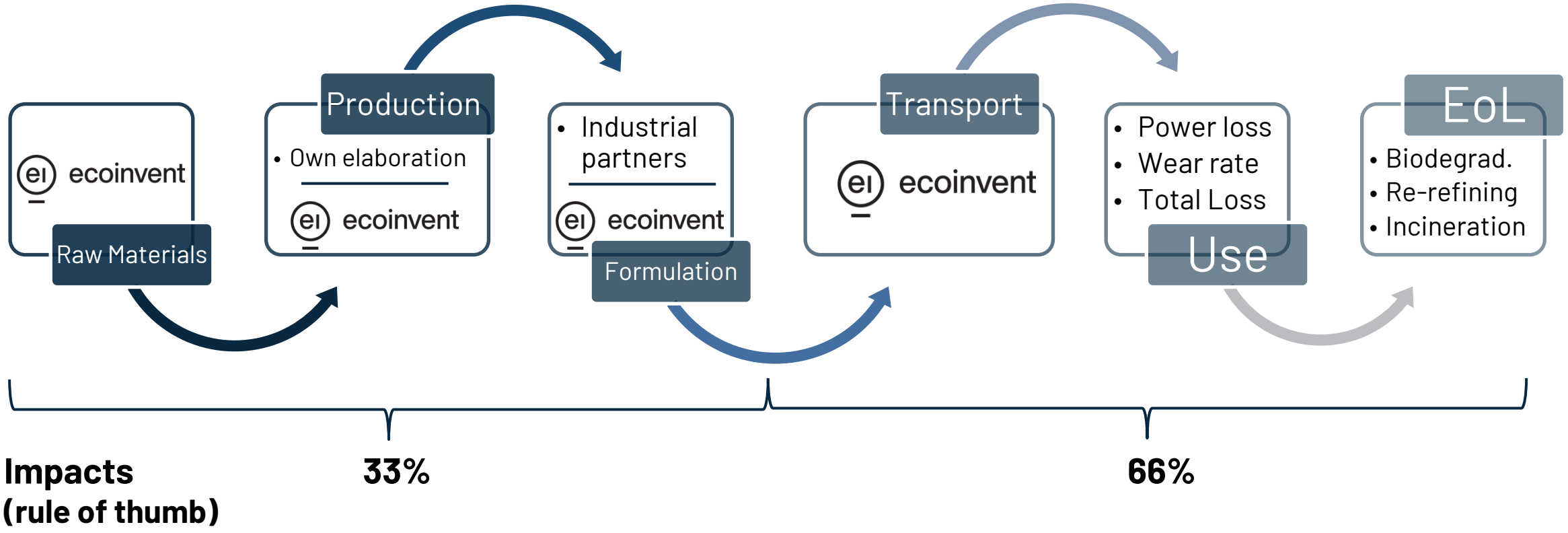

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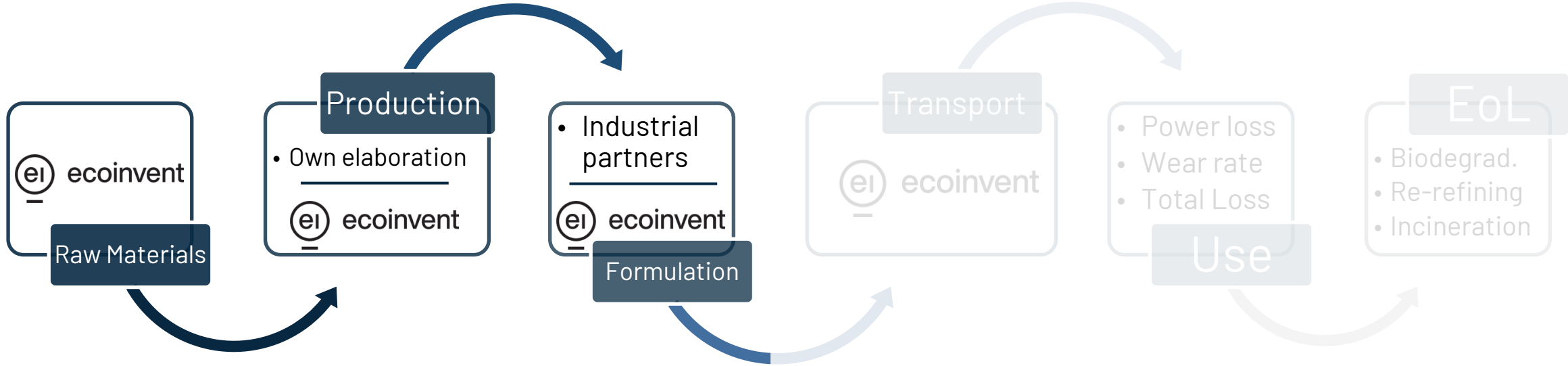

Impacts (rule of thumb)

33%

66%

SSbD base case

SSbD alternative

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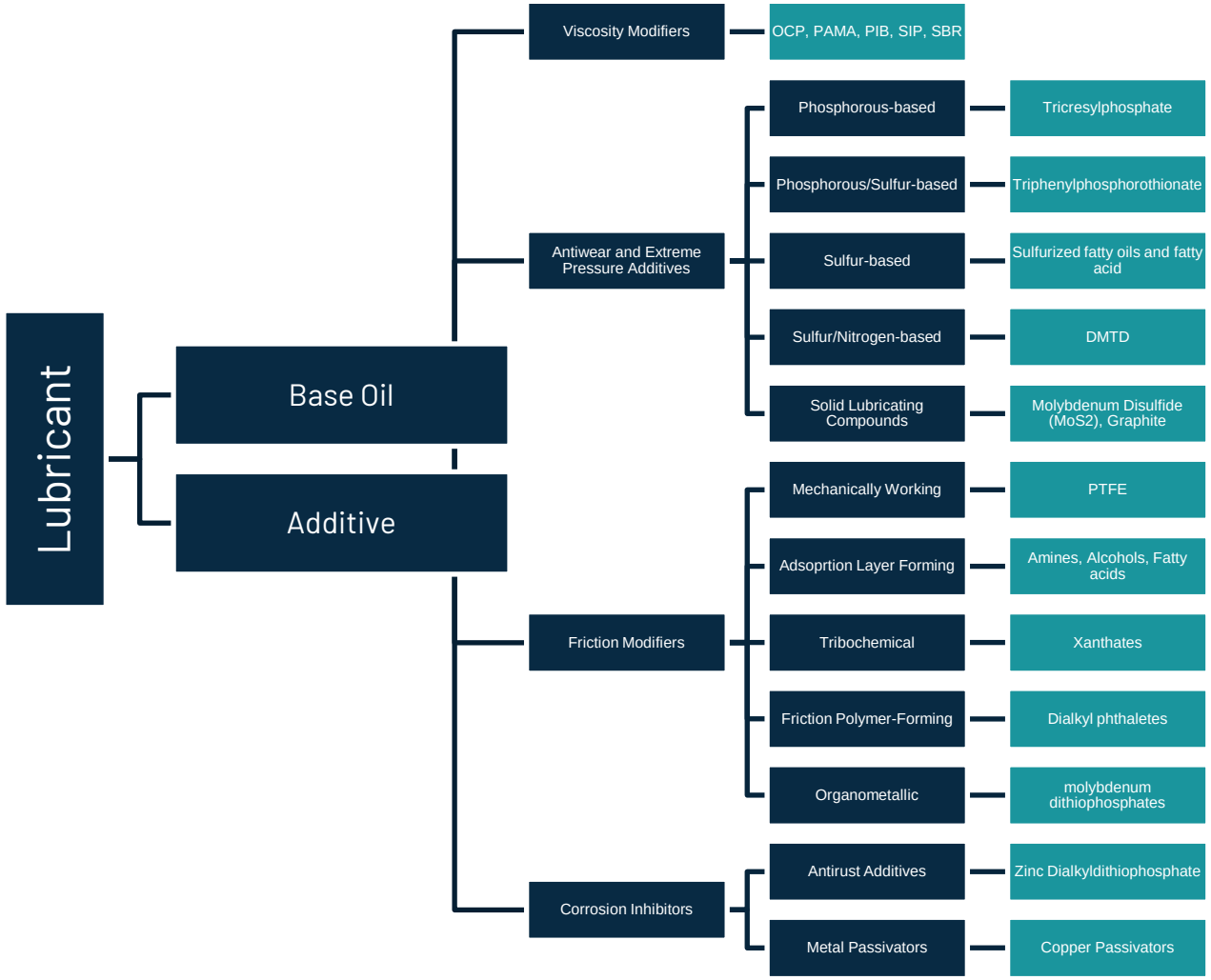
Raw Material Extraction and Production:
118 key chemicals have been identified and classified



The user will be allowed to selected an SSbD base case (to be substituted compound)

SSbD base case

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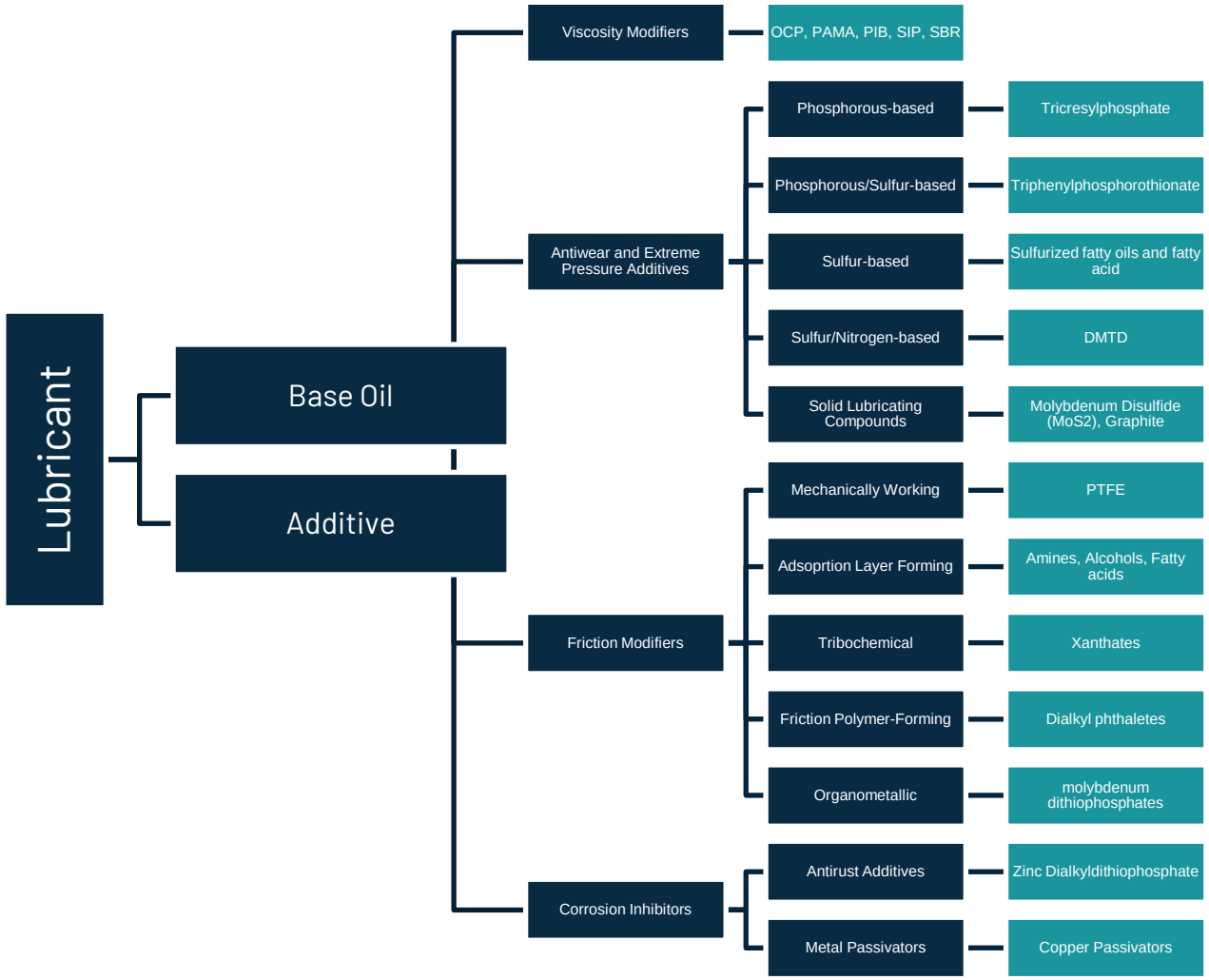
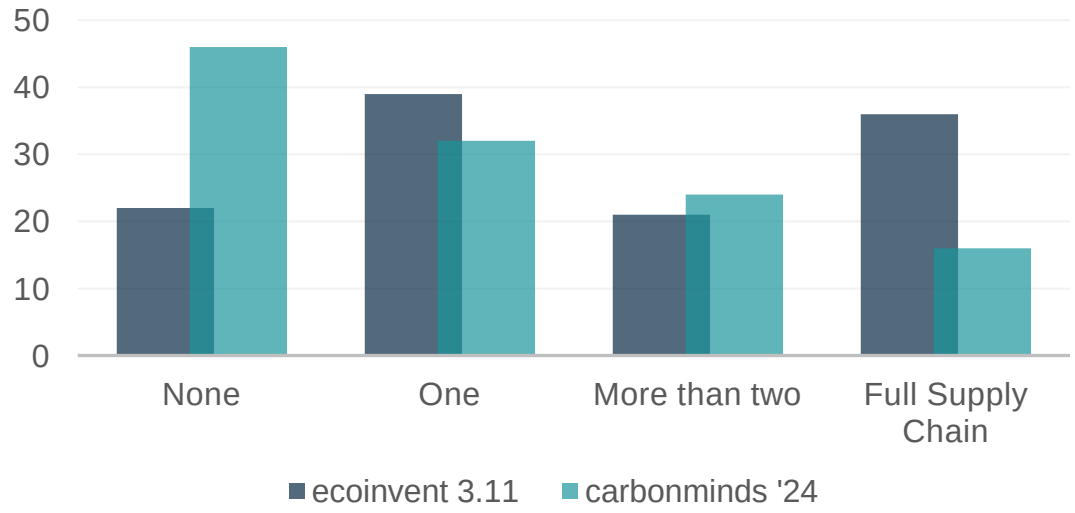


ecoinvent 3.11 vs. CarbonMinds´24:

Modelling steps necessary



Model myself (fill data gaps)

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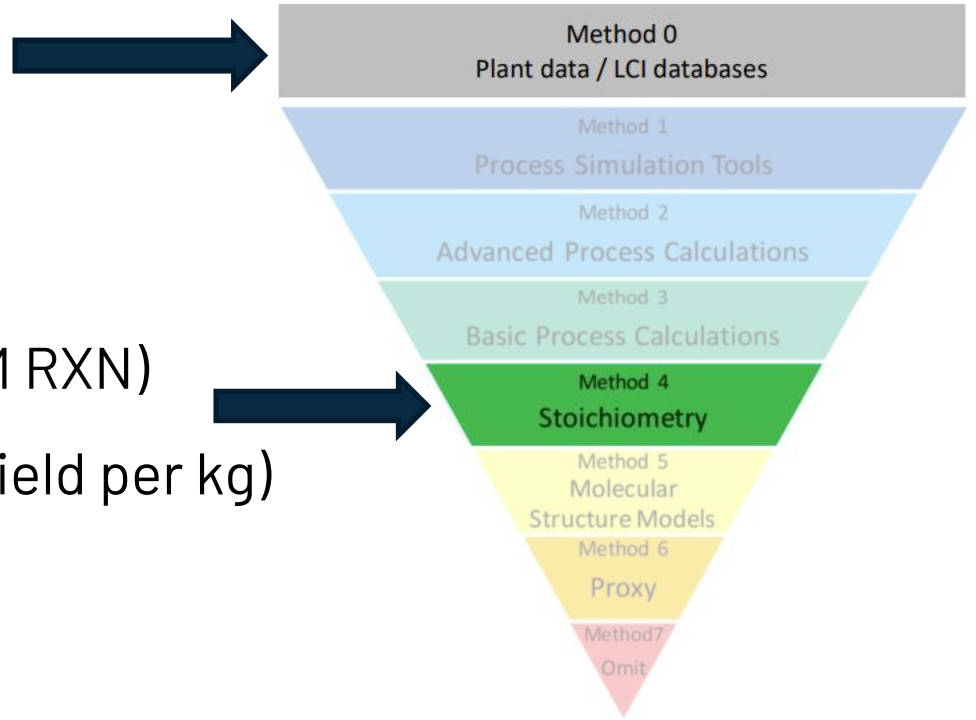
Raw Material Extraction and Production: How to fill data gaps? Also, for SSbD alternatives

- Use literature LCI from plant data
- Use ‚stochiometric approach'
  - Consult literature for routes (Ullmann, patents)
  - **Retrosynthetic tools in openLCA** (AIZynthfinder, IBM RXN)
  - Add „Gendorf Approx." (2.2 MJ , 0.4 kWh , 95% yield per kg)



Gendorf Approach from: Hischier *et al.*, *Int. J. LCA*. **2005**, *10(1)*, 59 – 67.

Parvatker *et al.*, *ACS Sus. Chem. & Eng.* **2019**, 7(1).

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Raw Material Extraction and Production: ‘Gendorf Approach’ in openLCA

Inputs/Outputs - Chemical Production Gendorf

Inputs

Flow	Amount	Unit	Provider
heat, district or in...	1.88647	MJ	market group f...
electricity, mediu...	0.39906	kWh	market group f...
heat, from steam, ...	0.20781	MJ	market for heat,...
Water, cooling, un...	0.01471	m3	
Water, river	0.00097	m3	
Water, well, in gro...	0.00082	m3	
chemical factory, ...	4.0000...	Item(s)	chemical factor...

Outputs

Flow	Amount	Unit	Provider
chemical produc...	**1.00000**	**kg**	
wastewater, average	5.58244...	m3	market for was...
wastewater, average	2.27712...	m3	market for was...
Water	0.00147	m3	
Water	0.01504	m3	

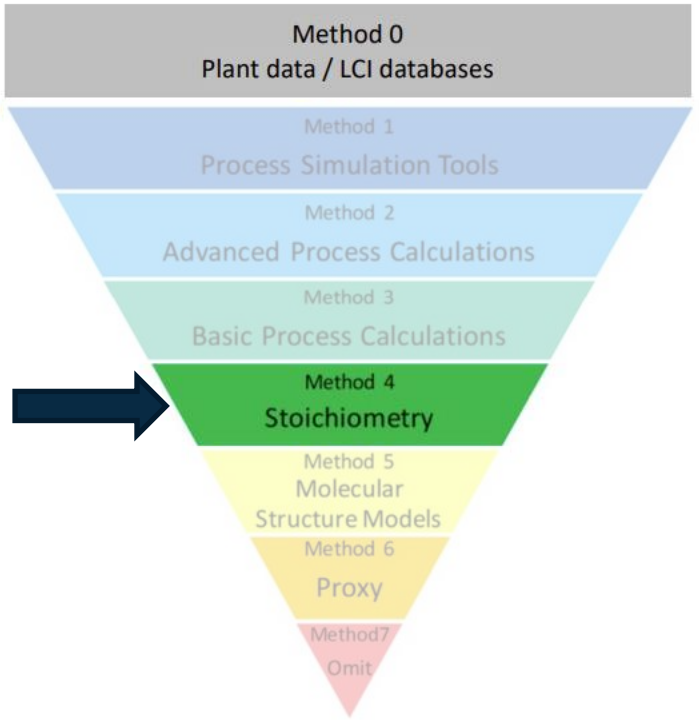
Inputs/Outputs - benzotriazole production - RER

Inputs

Flow	Amount	Unit	Provider	Da
chemical production	1.00000	kg	Chemical Pro...	
nitrous acid	8.40*1.0...	kg	nitrous acid p...	
o-phenylene diamine	8.40*1.0...	kg	market for o-...	

Outputs

Flow	Amount	Unit	Description
benzotriazole	**1.00000**	**kg**	**8.40 mol**
Carbon dioxide, fo...	0.05*((6*...	kg	In addition, ...



→ **Specific (esterification) or generic approach to describe reactions(ester+alcohol)**
→ **We are in the process of automating those steps (retrosynthesis in openLCA)**

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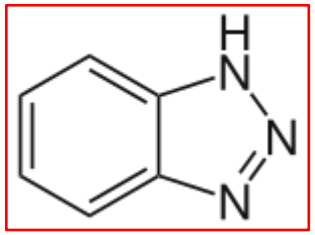
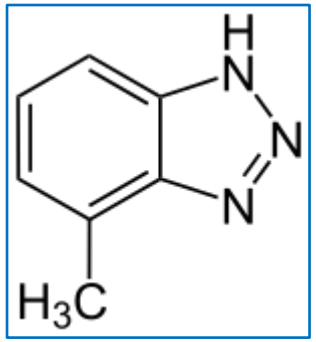
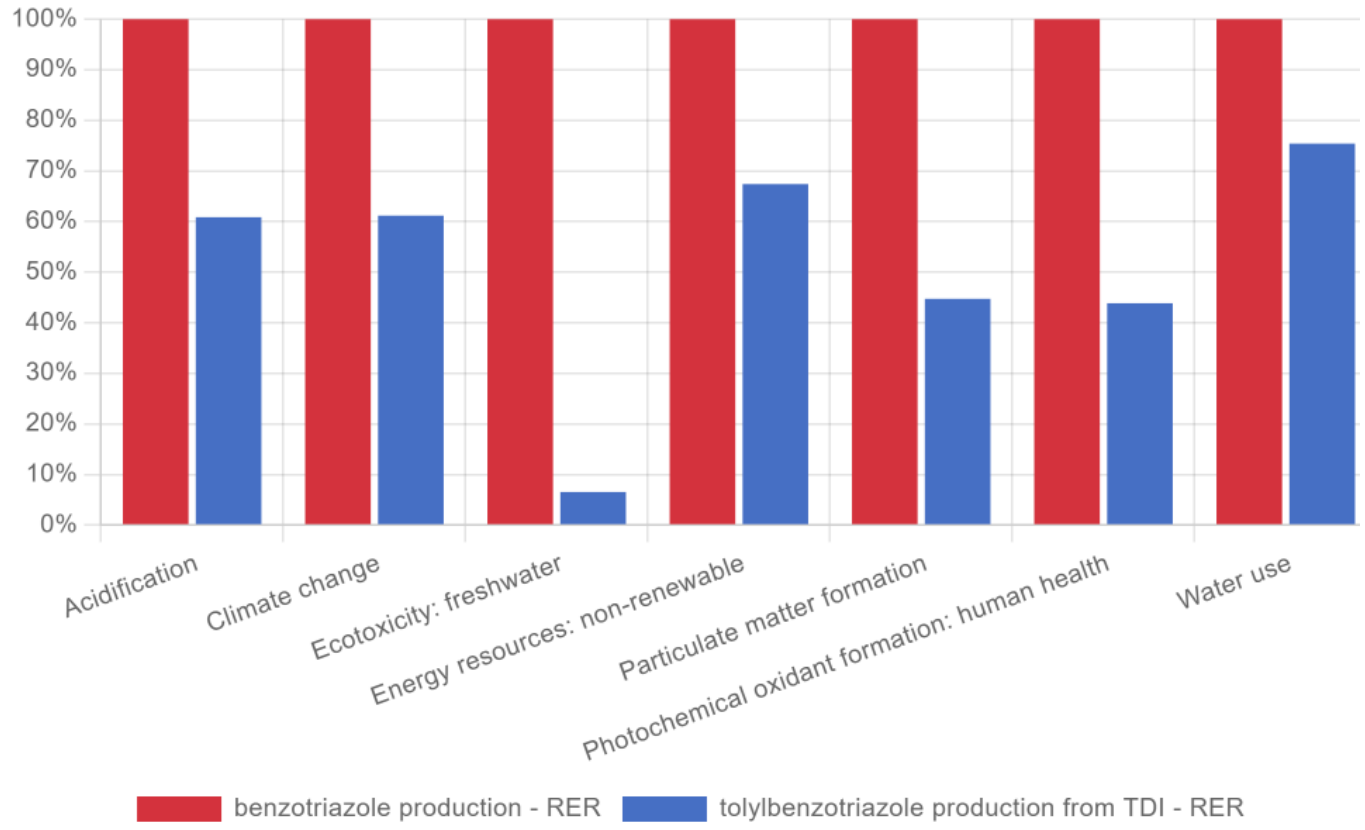
Raw Material Extraction and Production: The case of tolyltriazole (cradle-to-gate)



SSbD base case



SSbD alternative



cradle-to-gate, referenced to 1 mol of product, ecoinvent 3.11, EF 3.1 LCIA

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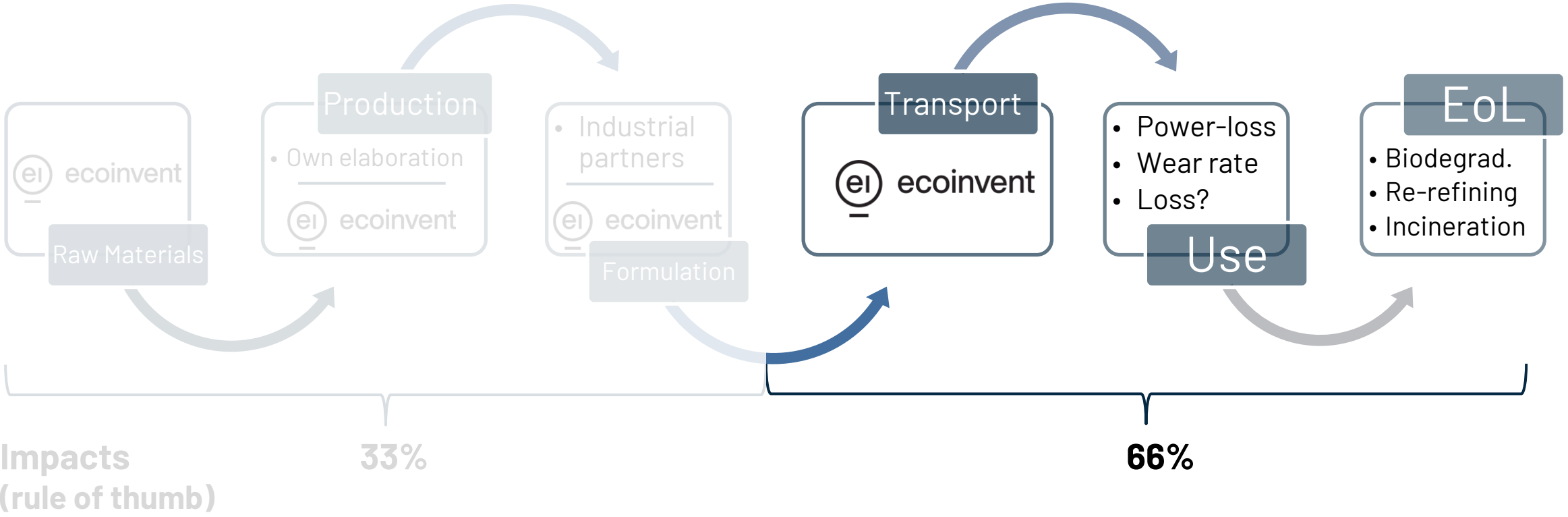
The Challenge:
Predict LCA for the entire life cycle



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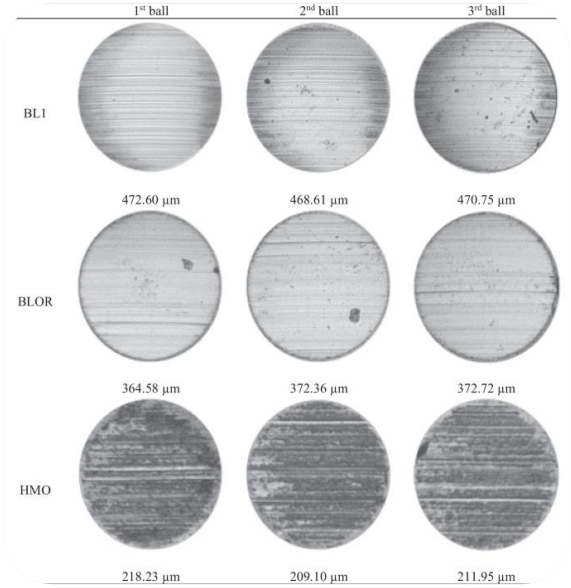
Use Phase:
How to get ‘performance’ into LCA?



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. E*nvironmental life-cycle assessment (LCA) of lubricants* **2013** *Biolubricants*, 527–564.

Wear protection (life time)

Oxidative stability (drainage intervals)

Power loss (Performance FU)

What has been done so far?

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Use Phase:
Classical functional units for LCA of lubricants (n = 20, 1999-2024)

Year	functional unit	Scope	Application	Performance Assessed?
2012	1 kg of final product	Cradle-to-Gate	Base oil and fully formulated engine oil	per kilogram of product and per kilogram adjusted to the lifetime
2013	1 kg of oil	Cradle-to-Gate	Chainsaw oil	Lubricant consumption
2018	400 holes	Cradle-to-Gate	Drilling	Reduced power consumption

Integration of the **performance** into the **functional unit**:

A. The **consumption** of the lubricant itself → **hard to simulate** (~~fixed lubrication~~)

B. **Adjustment** of the **lifetime** of the function (kilometre-adjusted) → **Wear**

C. By taking the **reduction of power consumption** (here pumping) → **Power loss**

- Hence, **reduction of power generation** can be taken into account

We are developing multiple functional units to align with the specific needs of various application scenarios

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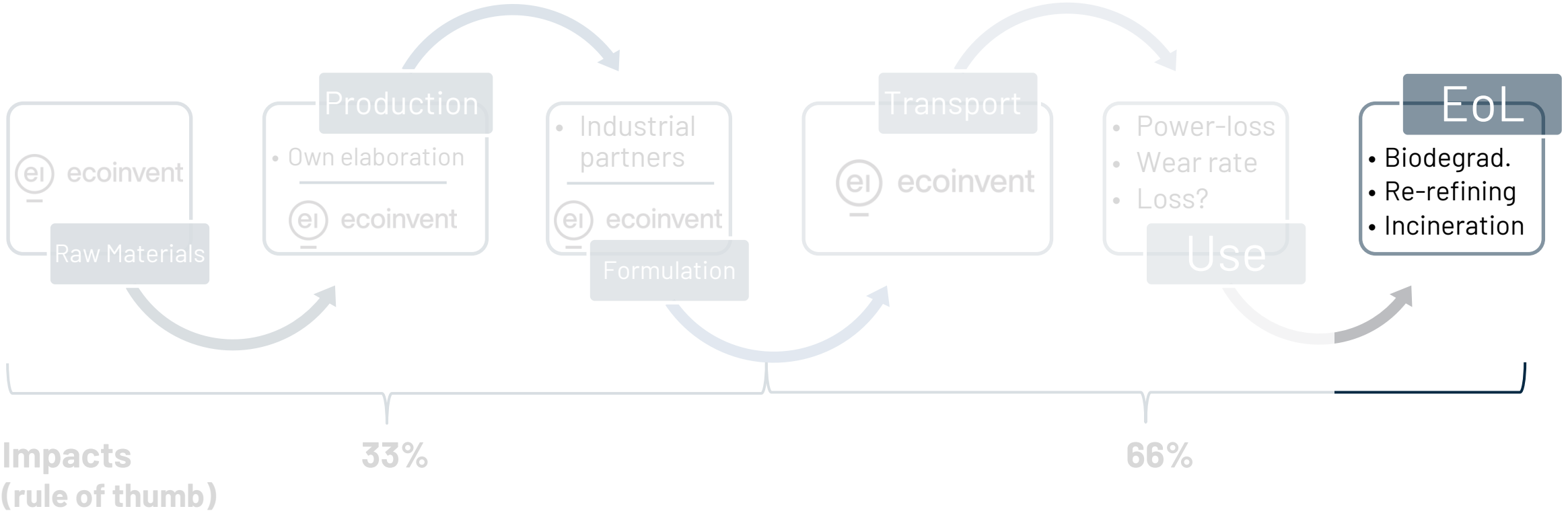
The Challenge:
Predict LCA for the entire life cycle



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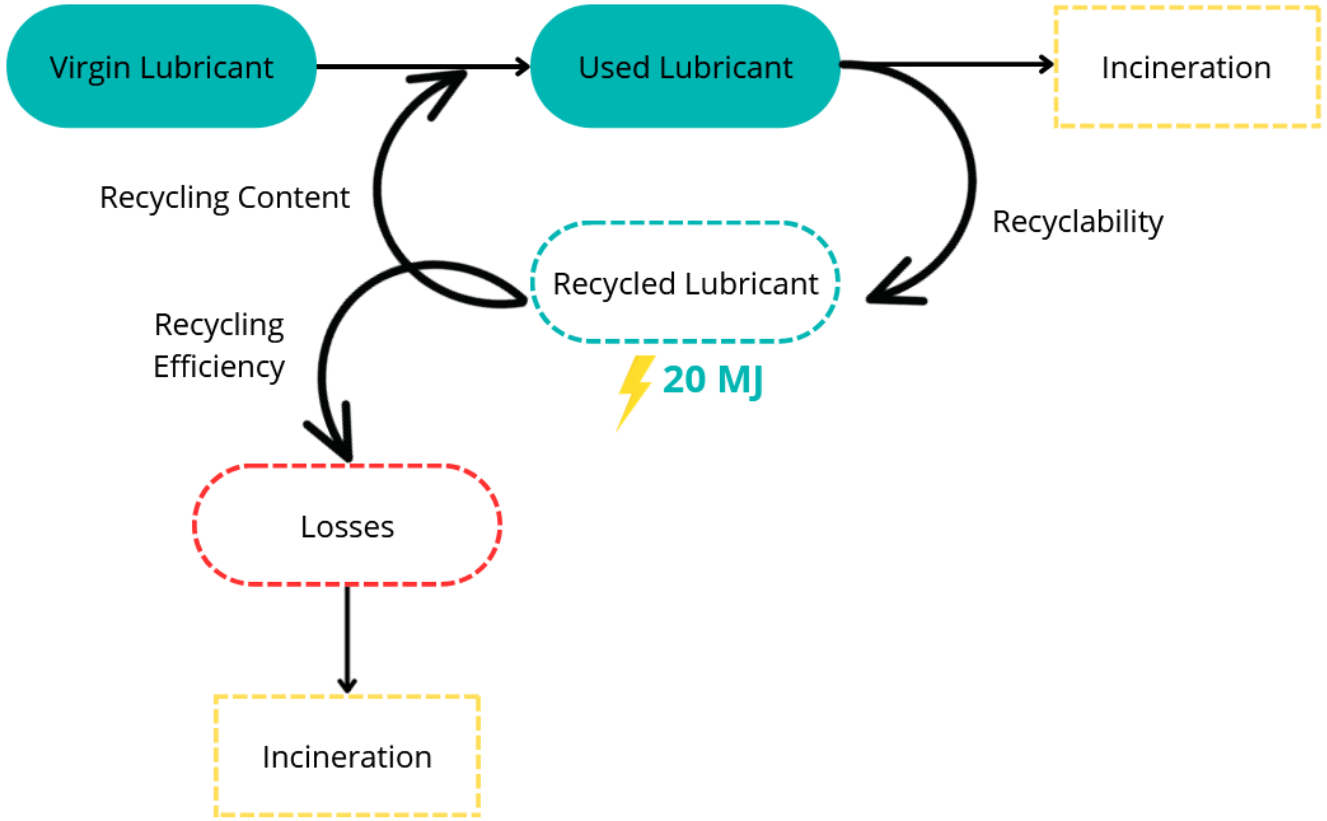
End-of-Life:
How to simulate EoL of lubricants?



*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.*

EoL of lubricants is quite diverse:

- Re-refining, loss, littering and incineration
- To **predict the EoL** of lubricants and their components, we will use **EWC and simul.**:
  - User information or **AI** selection
  - Thermo-oxidative stability (**rMD**)
  - Biodegradability (**QSAR**, simplified)

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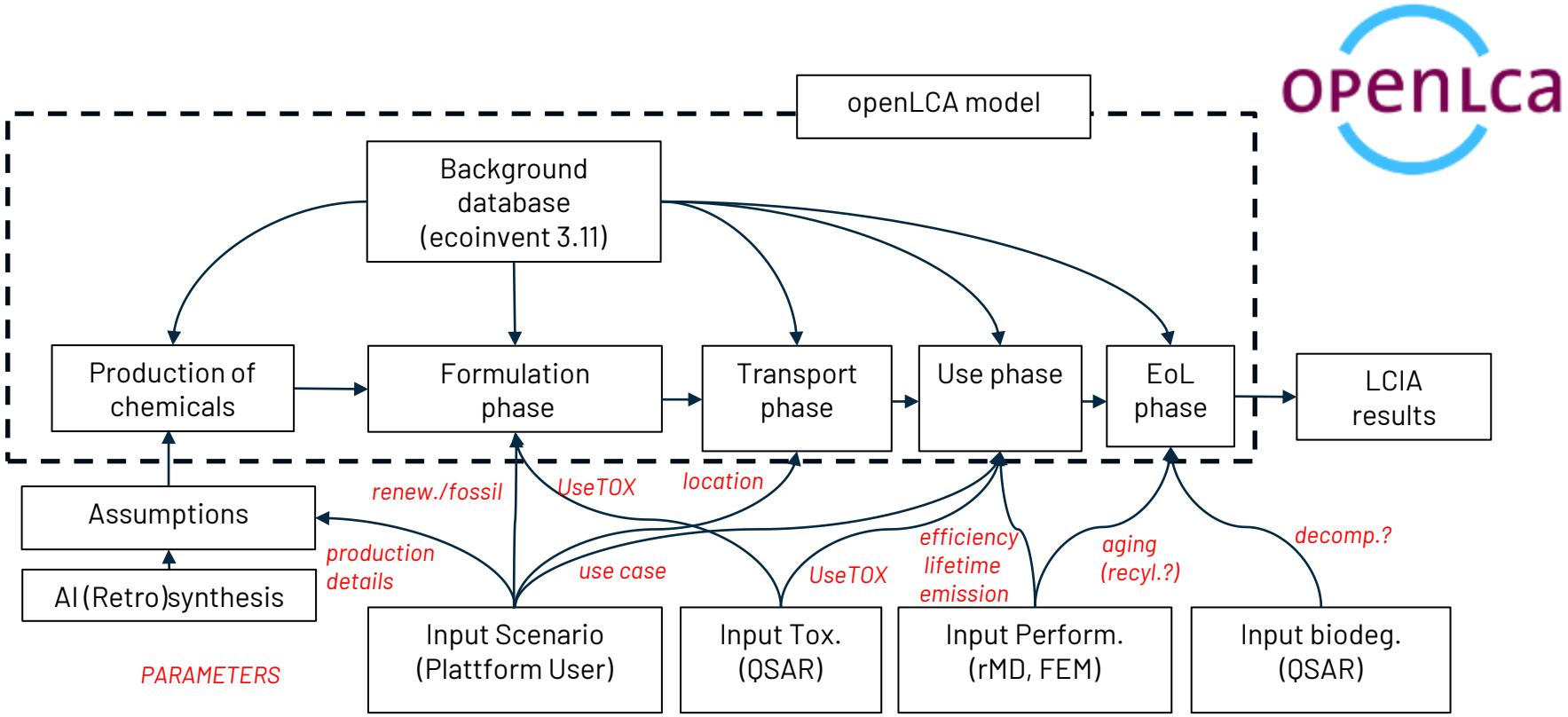
FÚLL LIFE CYCLE WITH PARAMETERS



Parametrized LCAs allows fully integrated SSbD approaches

→ openLCA's API will allow platform/AI interaction

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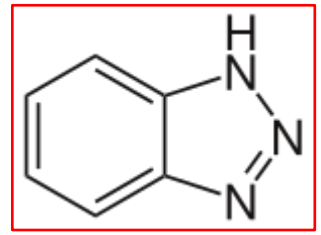
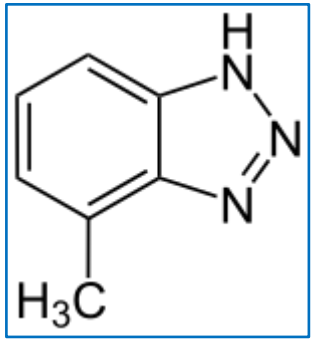
Main challenges and what's next?

- **SiToLub** simulates and integrates **safety, sustainability** and **performance**
- Accelerate the update of **SSbD** into **early development** phase **with tools**
- Deriving impacts from **SMILES** through **scenarios**
- Production phase from **existing data** and **retrosynthesis**
- **Use** phase should **not be overlooked** in **SSbD** (**case-by-case FU**)
- End-of-Life might be predicted (EWC codes, **biodegradability, re-refining**)



SSbD base case



SSbD alternative

Future development:

- Integration of **data quality (MCS)** and **prospective LCA**
- Progress of the **socio-economic assessment** (Step 5, SSbD)

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Thank you!

Jonas Hoffmann
GreenDelta GmbH
hoffmann@greendelta.com

Step 5: Socio-economic assessment

5.02.P-Mo431 - Comparative Assessment of Early-Stage social and critical raw material asssesment in the SSbD Framework: Addressing current generic Databases

Ashrakat Hamed, Jonas Hoffmann and Andreas Ciroth, GreenDelta GmbH, Germany

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