SITOLUB

SITOLUB

SIMULATION TOOLS FOR THE DESIGN OF SAFE AND SUSTAINABLE LUBRICANTS

Holistic Sustainability: Safe & Sustainable by Design

GreenDeLTa

Dr. Jonas Hoffmann

OpenLca

Pre-Congress Seminar at the 60th
UEIL Annual Congress

Co-funded by the European Union

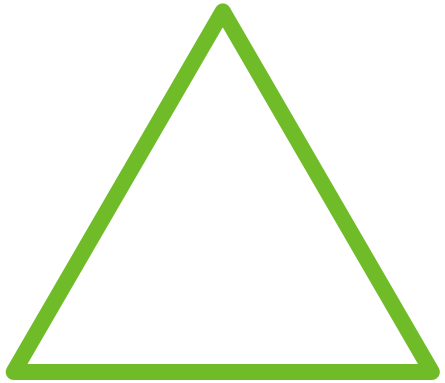
Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

GreenDelta background

- Founded by Dr. Andreas Ciroth in 2004, Berlin; now ~ 25 employees (engineers, developers etc)
- Business world-wide: sustainability research, product carbon footprinting, **life cycle assessments**, databases, software for life cycle assessments and sustainability, environmental product declaration

Sustainability consultancy and research

environmental LCAs, resource criticality, social LCAs, LCC



Database development and distribution

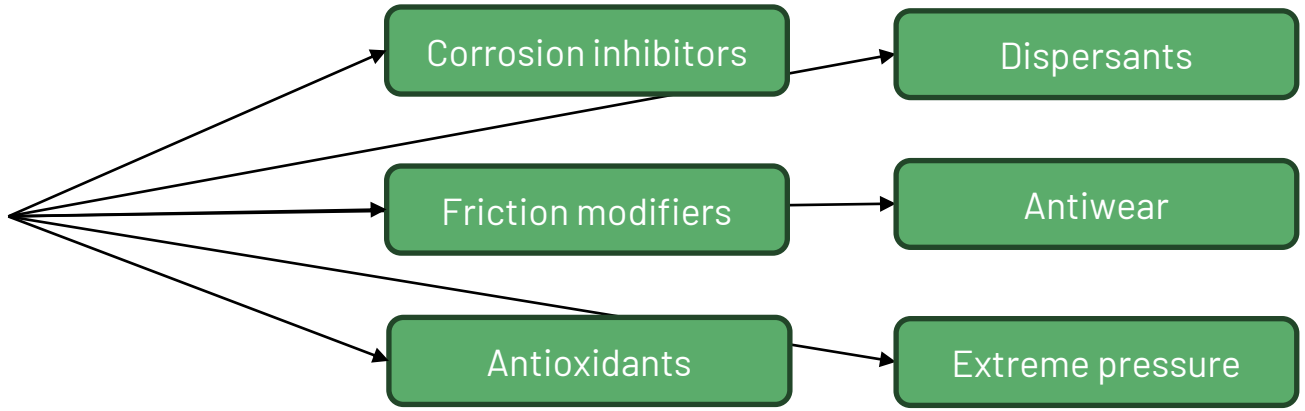
Software development, especially open source

Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

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

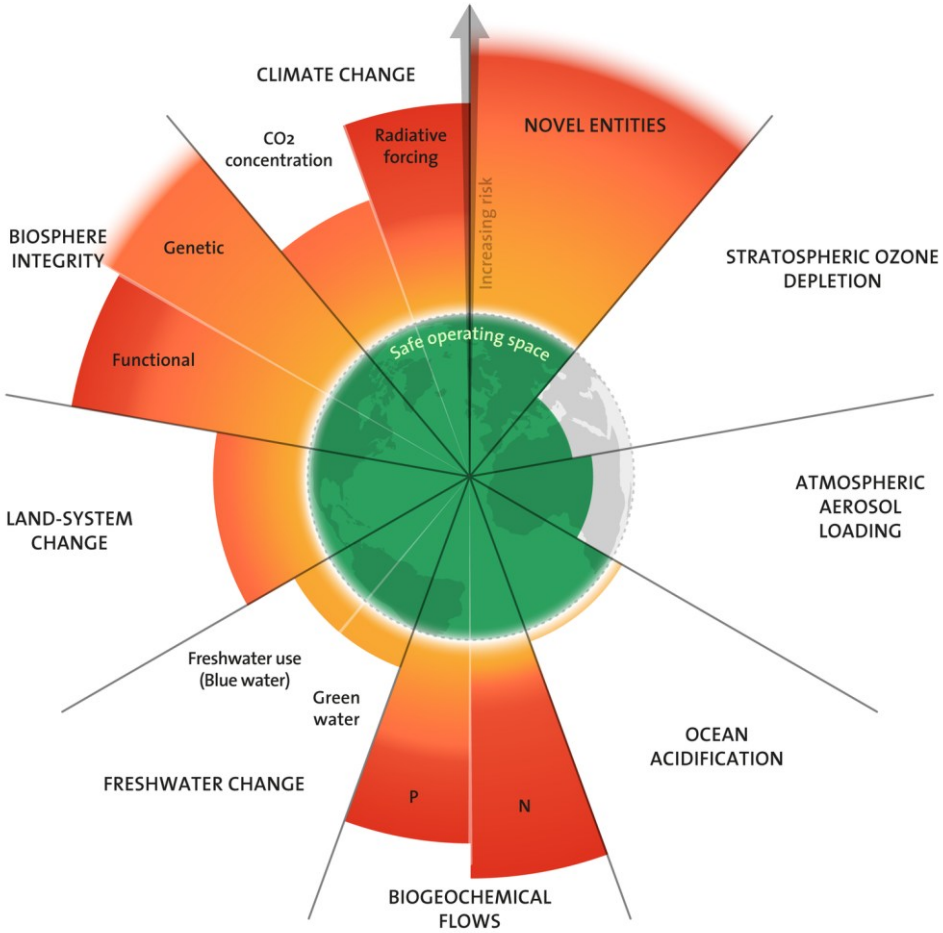
BLAUER ENGEL DAS UMWELTZEICHEN

Industry is in need for novel safe and sustainable solutions!

Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

The planet is already at its limit



9 boundaries assessed,
7 crossed

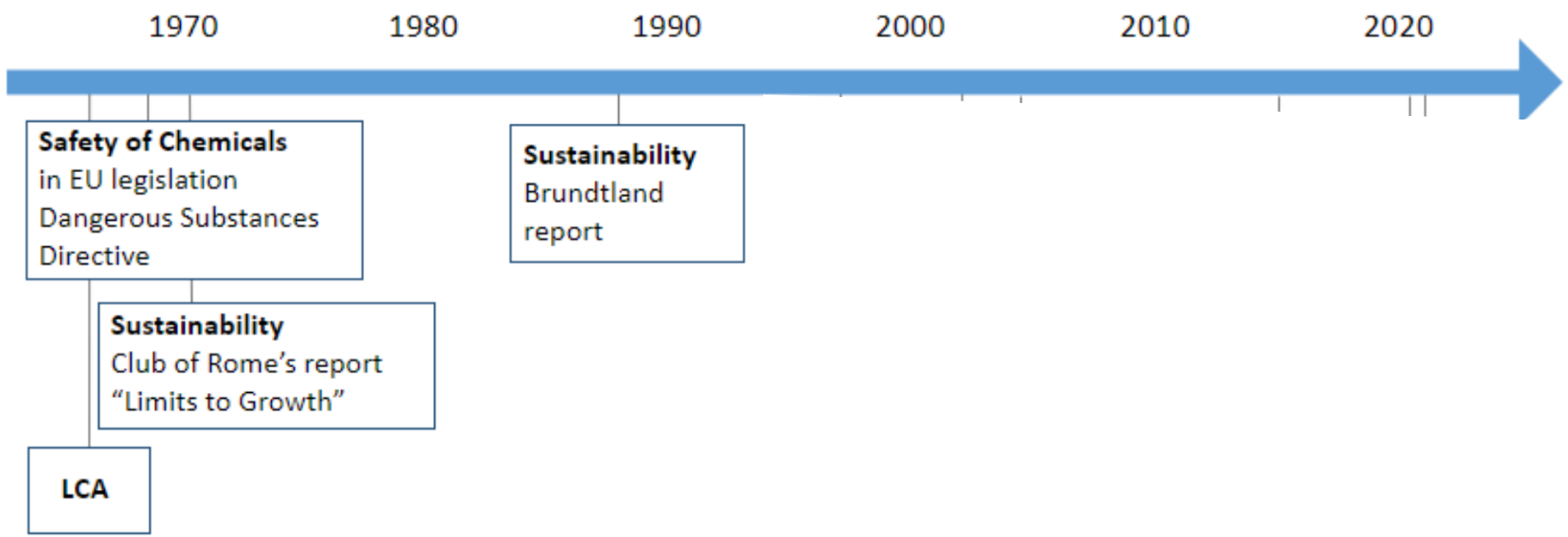
'With such an enormous percentage of untested chemicals being released to the environment, ***a novel entities boundary*** *defined in this manner is* ***clearly breached****.'*

Sakschewski and Caesar et al. 2025, Rockström *et al.*, *Sci. Adv.* **2023**, 9, DOI 10.1126/sciadv.adh2458.

Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

So how to safely innovate chemicals?



*'The SSbD framework promotes such a **holistic approach** that integrates **safety and sustainability** of chemicals, materials, products and processes throughout their **entire life cycle** and **minimizes** their **environmental footprint**.'*

Caldeira C., Farcal R., Moretti C., Mancini L., Rasmussen K., Rauscher H., Riego Sintes J., Sala S. Safe and Sustainable by Design chemicals and materials - Review of safety and sustainability dimensions, aspects, methods, indicators, and tools. EUR 30991 EN, Publications Office of the European Union, Luxembourg, 2022, ISBN 978-92-76-47560-6, doi:10.2760/879069, JRC127109

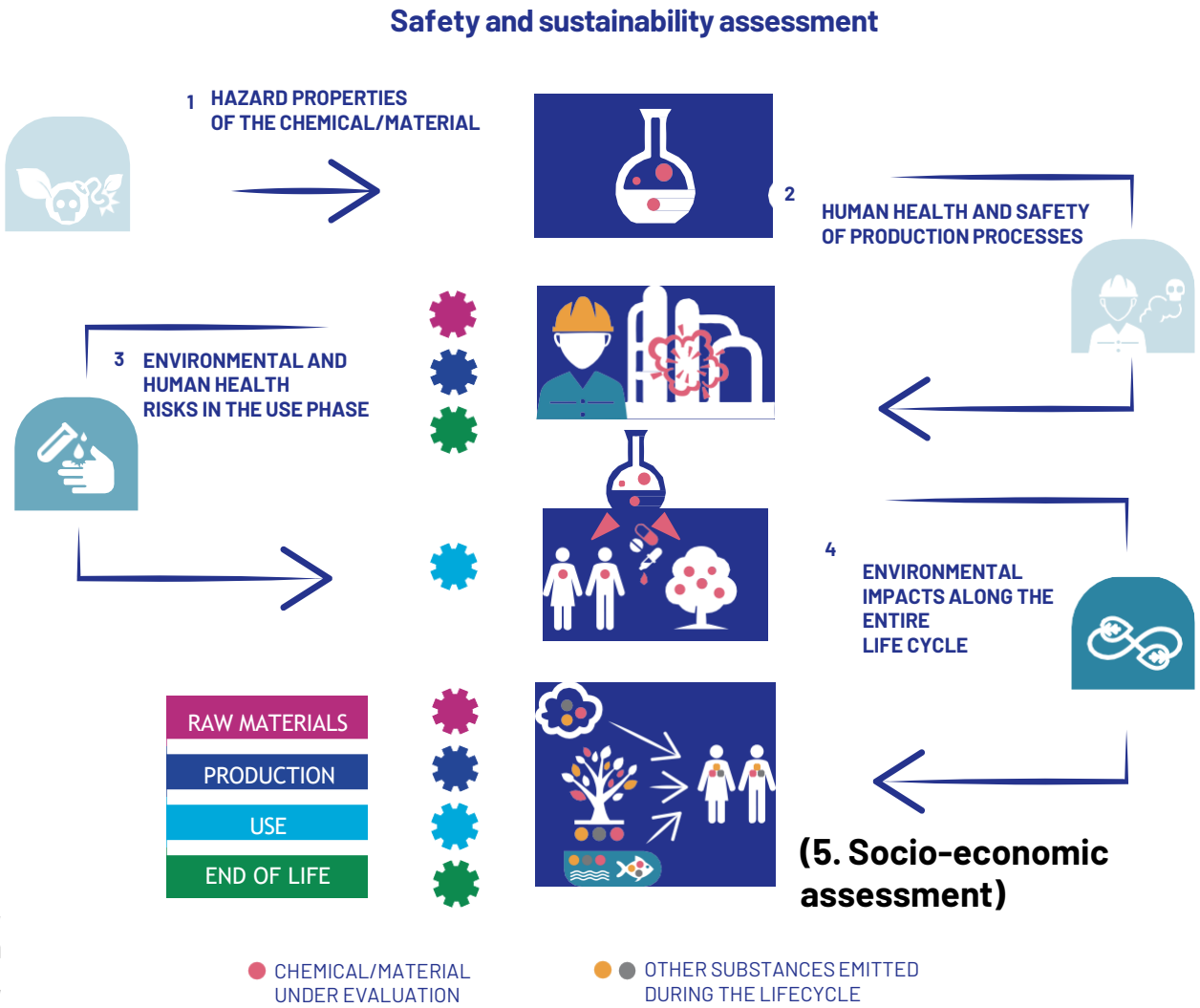
Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

Safe and Sustainable by Design

Design principles:

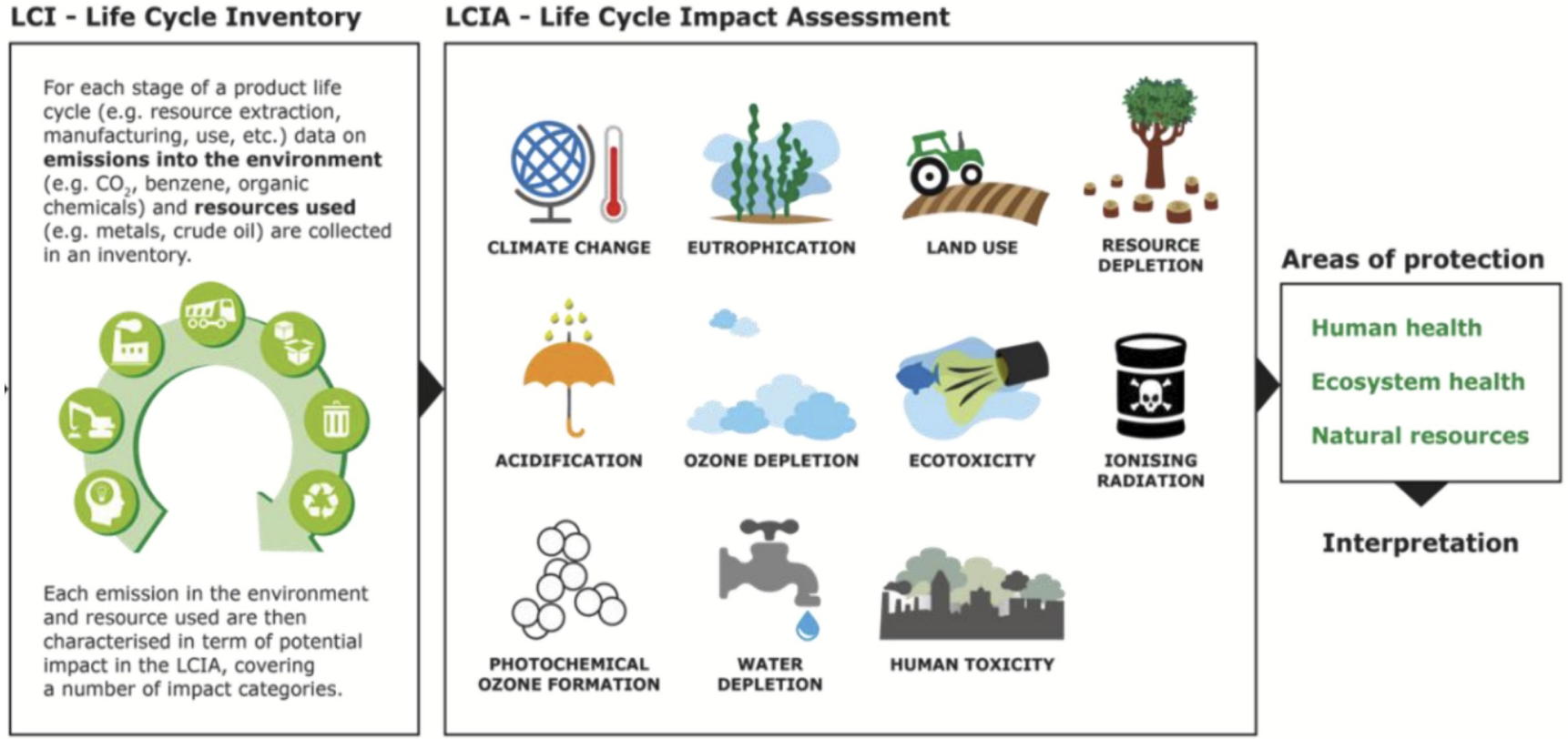
- Green chemistry
- Green engineering
- Sustainable chemistry
- Circularity by design
- Benign by design



European Commission, Directorate-General for Research and Innovation, Safe and sustainable by design chemicals and materials – A European assessment framework, Publications Office of the European Union, 2022, https://data.europa.eu/doi/10.2777/86120

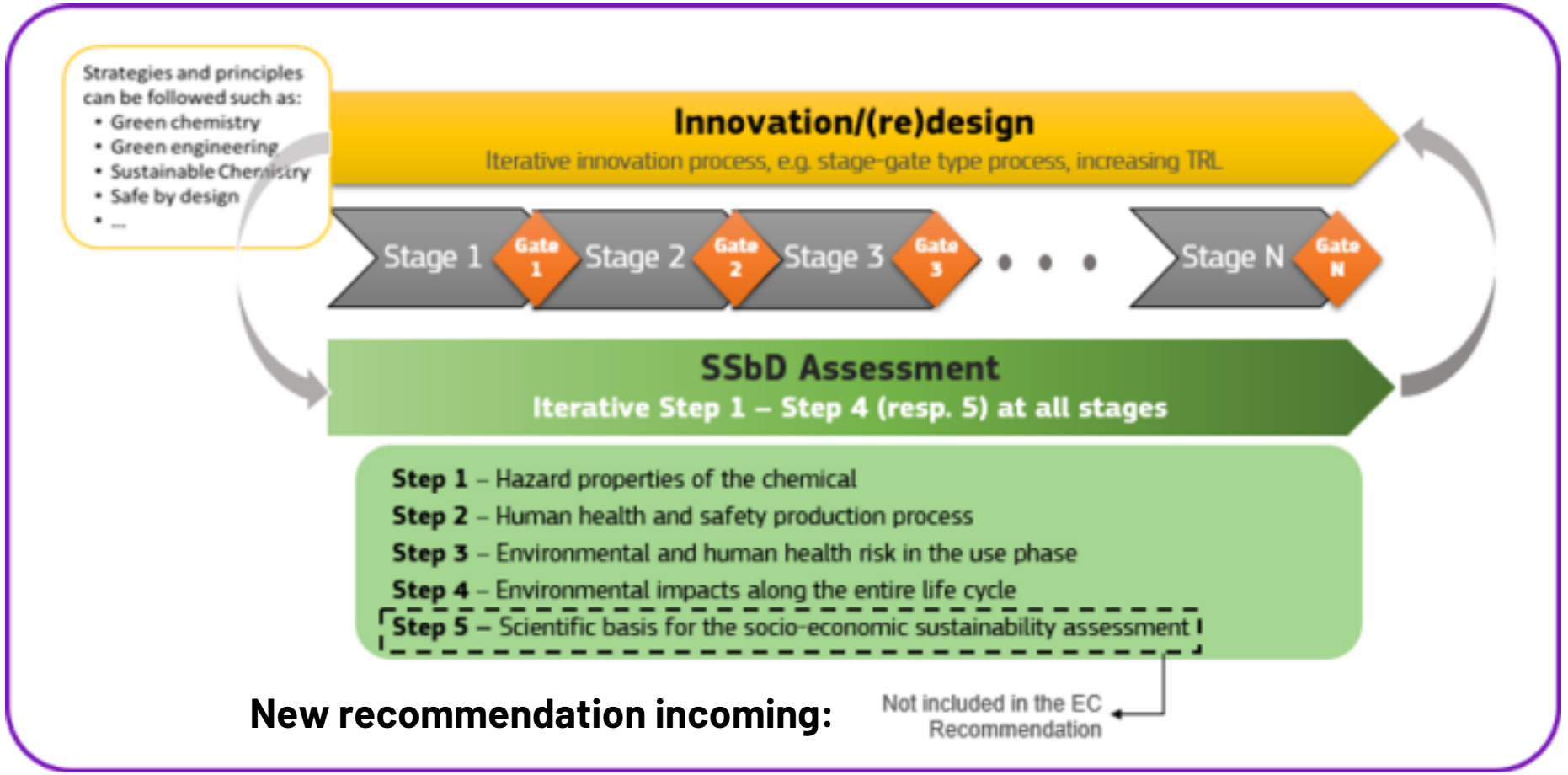
Life Cycle Assessment

Definition (DIN 14044): *'Life Cycle Assessment (LCA) is a compilation and evaluation of inputs, outputs and the potential environmental impacts of a product system through its life cycle.'*



Sala S., Cerutti A.K., Pant R., Development of a weighting approach for the Environmental Footprint, Publications Office of the European Union, Luxembourg, 2018, ISBN 978-92-79-68042-7, EUR 28562, doi:10.2760/945290

Safe and Sustainable by Design



https://joint-research-centre.ec.europa.eu/jrc-news-and-updates/designing-safer-and-more-sustainable-chemicals-and-materials-methodological-guidance-2024-07-11_en

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.

Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

THE PROJECT

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

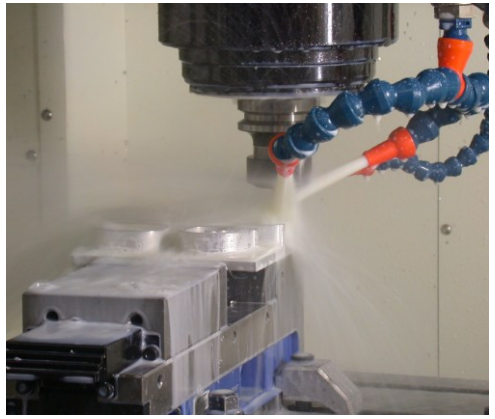
HORIZON Research and Innovation Action:
Computational models for the development of safe and sustainable by design chemicals and materials

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

Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

Use Cases

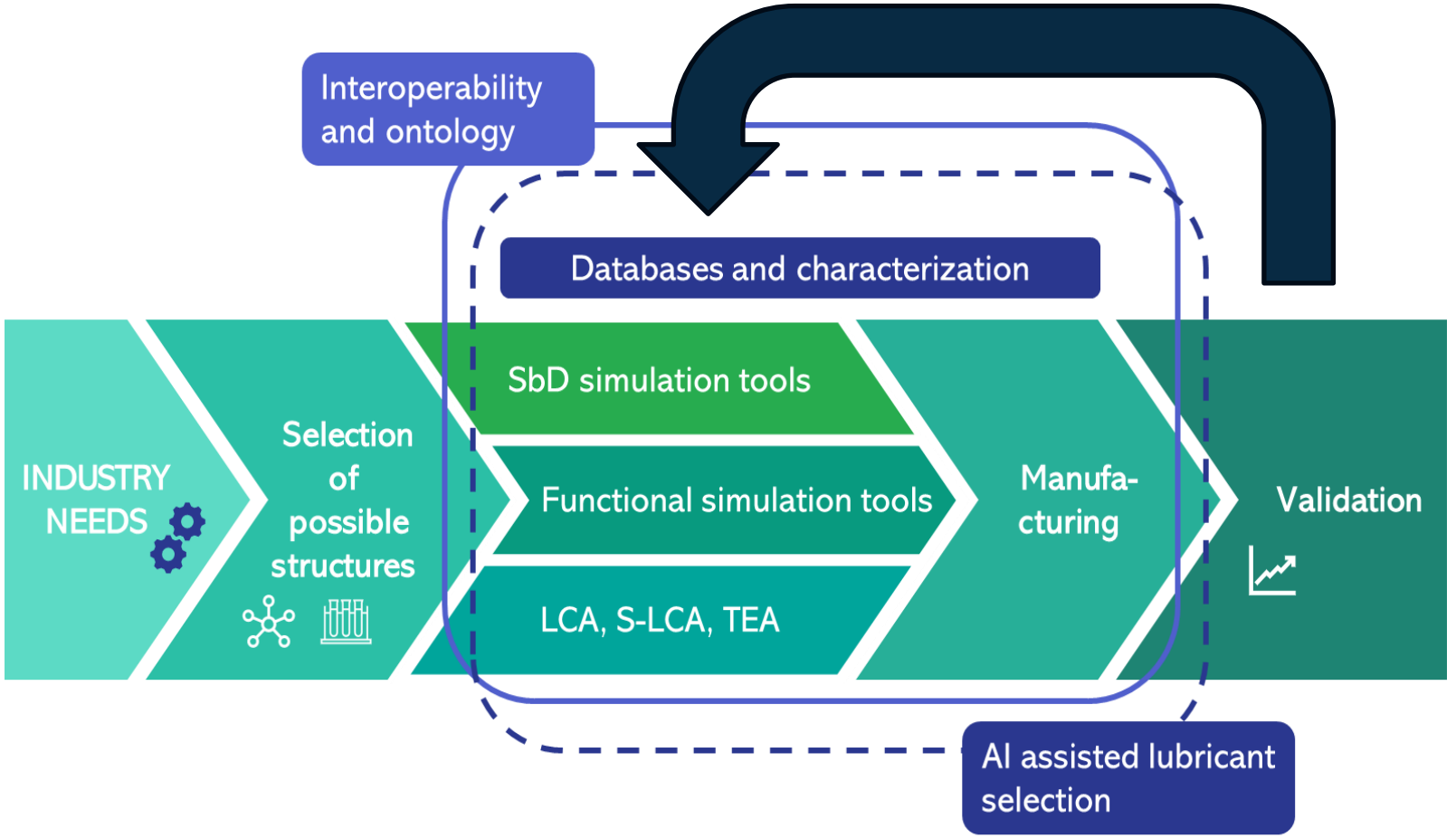


1. Metal-working fluids (chl. Paraffins)
2. Antiwear Additives (PTFE-based)
3. Corrosion Inhibitors (Benzotriazole)

Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

WORKING FLOW



Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

SITOLUB SIMULATION APPROACH

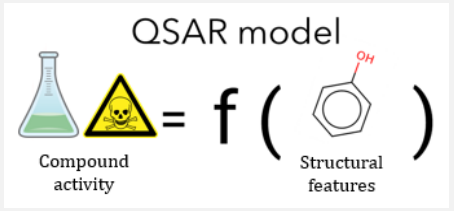
QSAR Simulation

Quantitative

Structural

Activity

Relationships

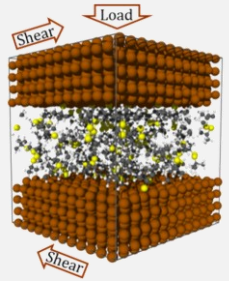


(Eco)Tox. & Biodegr.

Performance Sim.

- Evaluation for lubricants and their components

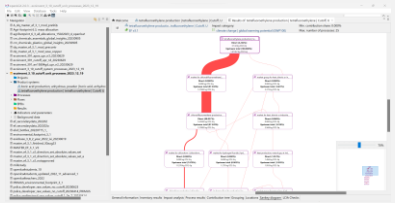
- Reactive MD simulation



Performance

Sustainability Sim.

- Environmental Impacts
- Social Impacts
- Economical Costs



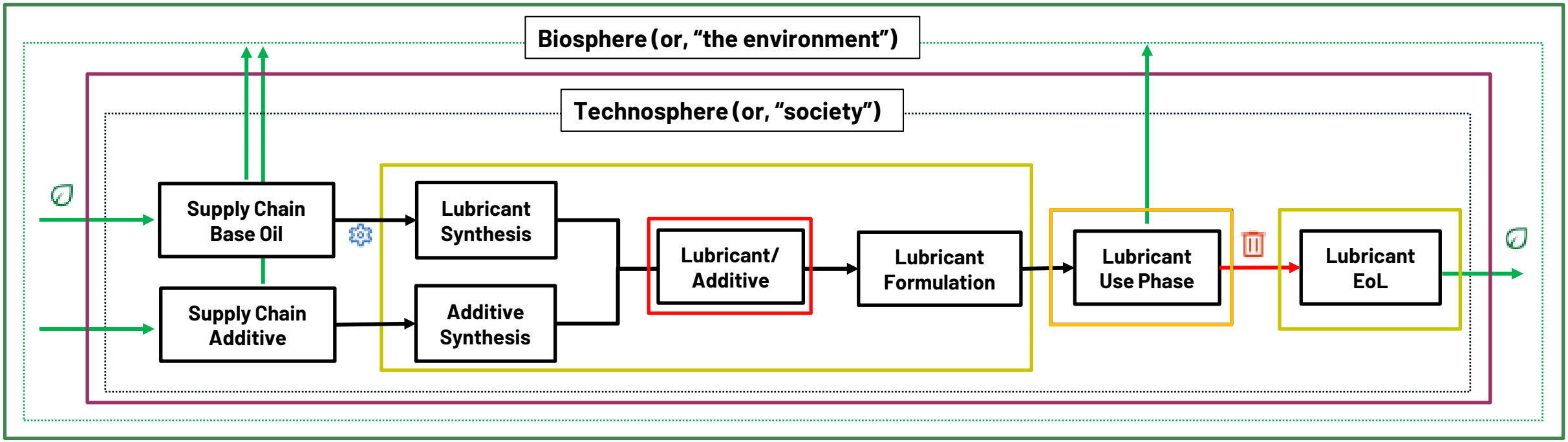
Sustainability

AI-supported lubricant selection and data synthesis

Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

SITOLUB SSbD FRAMEWORK

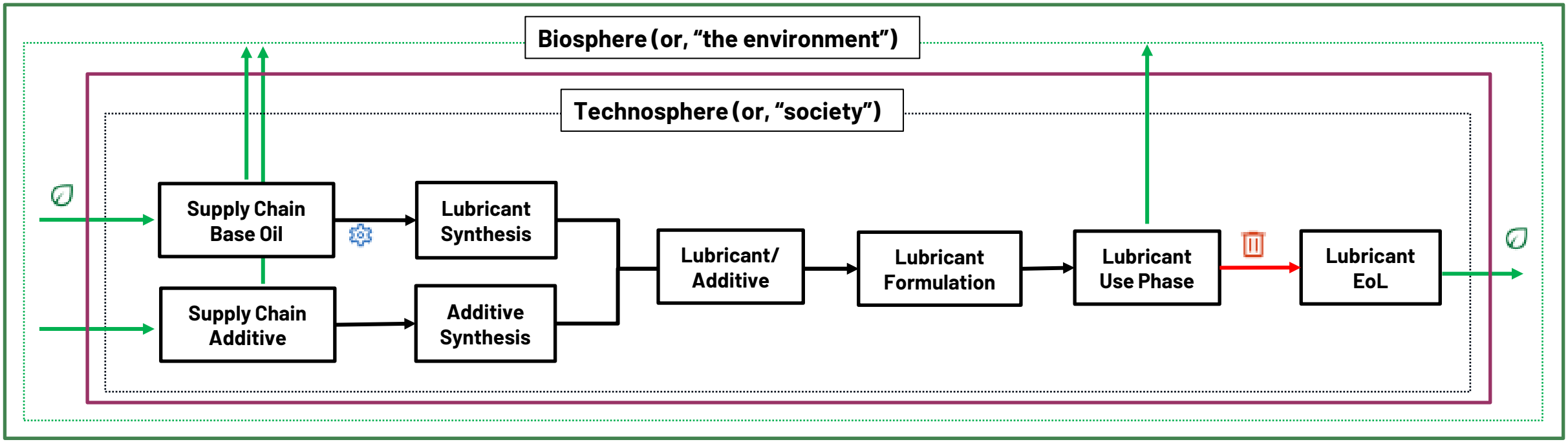


SAFETY:	Hazard Assessment	Risk Assessment during Processing	Risk Assessment in Application
SUSTAINABILITY:	Performance Assessment	Environmental Impact Assessment	Socio-economic Assessment

Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

SITOLUB SSbD FRAMEWORK



SAFETY:

SUSTAINABILITY: GreenDeLTa

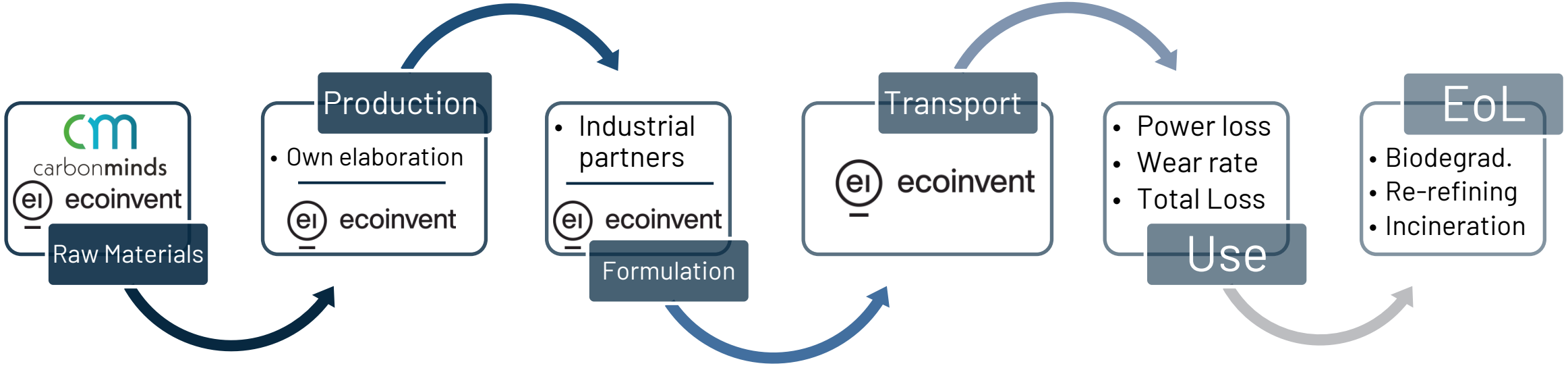
Environmental Impact Assessment

Socio-economic Assessment

Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

The Challenge:
Predict LCA for the entire life cycle



Impacts (rule of thumb)

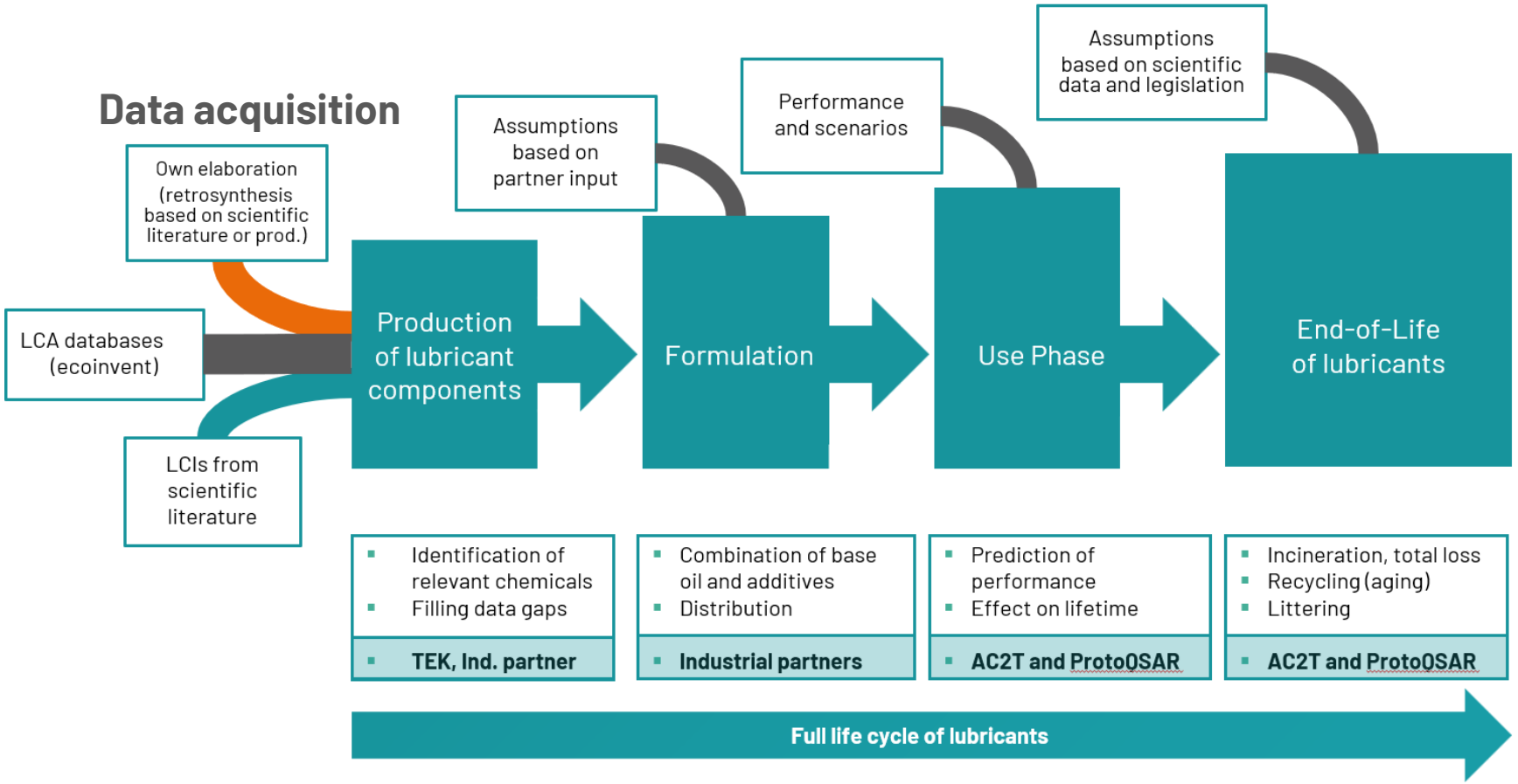
33%

66%

Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

The Challenge:
Predict LCA for the entire life cycle



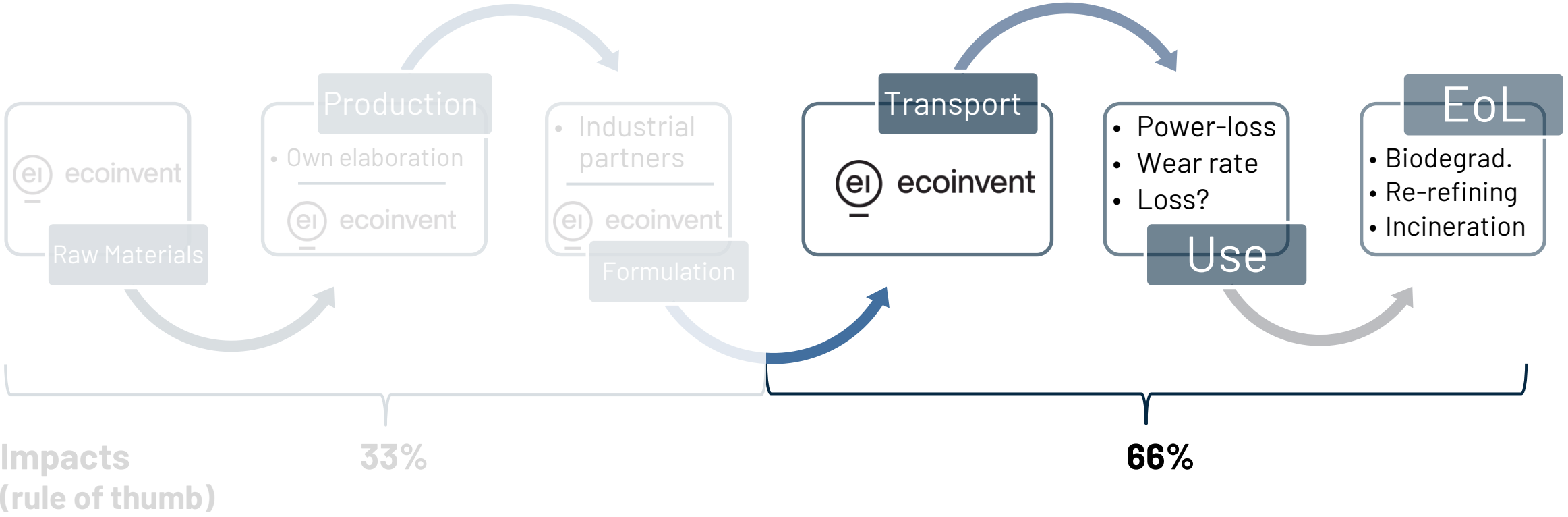
Various sources for LCIs and assumptions:

- Grey/White literature
- Background LCIs
- Expert knowledge
- Partner's input
- Other tools

Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

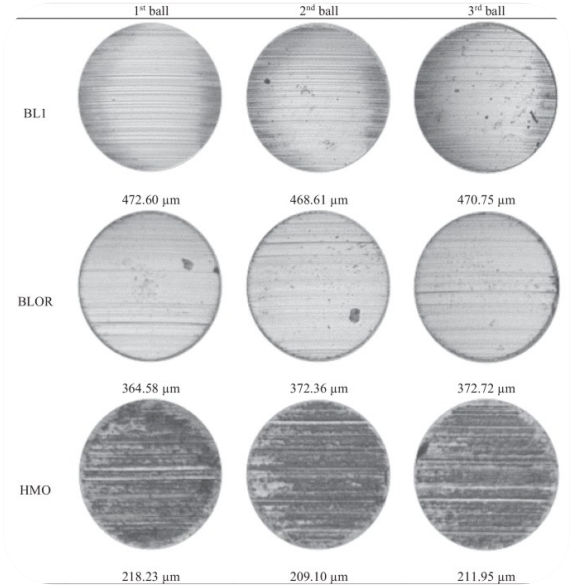
The Challenge:
Predict LCA for the entire life cycle



Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

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?

Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

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**

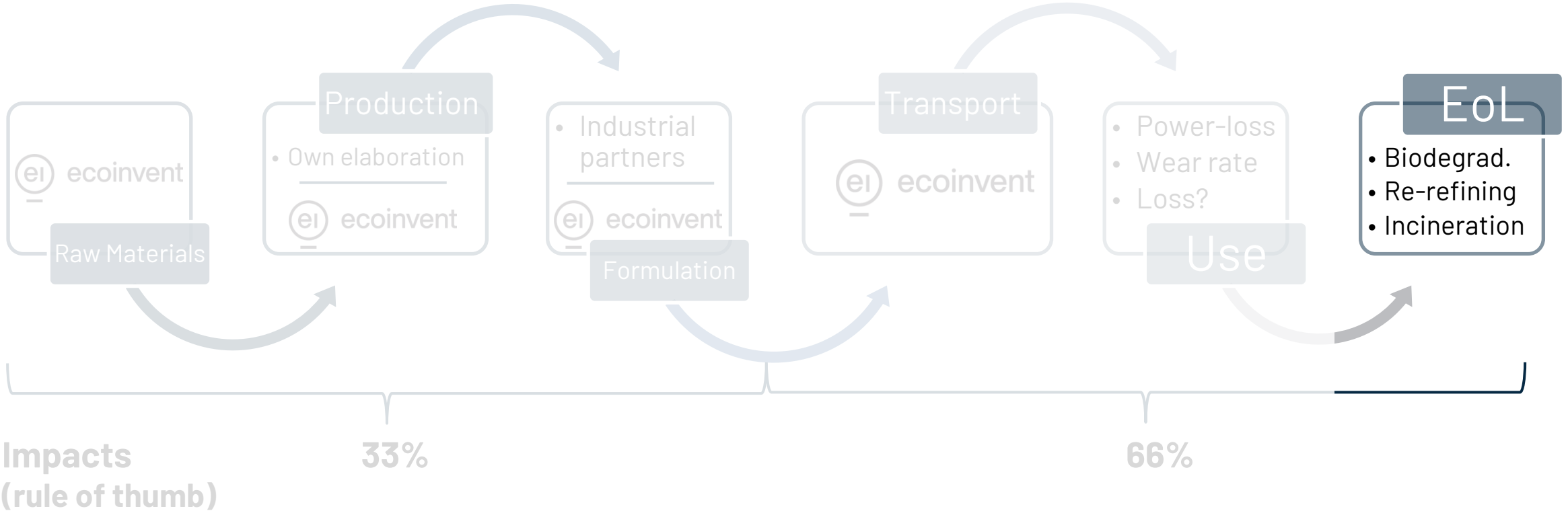
C. By taking the **reduction of power consumption** (here pumping) → **Power loss**

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

Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

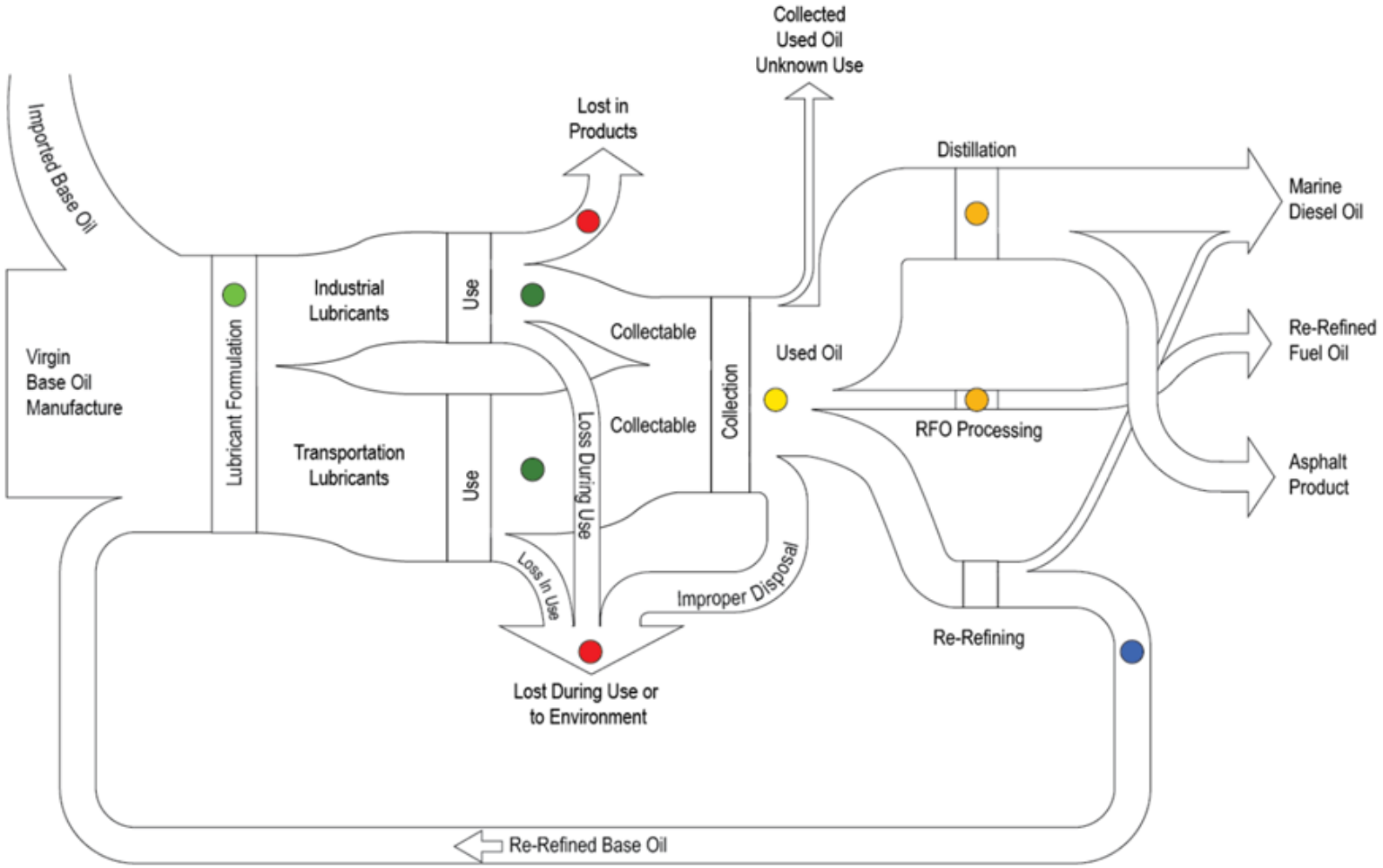
The Challenge:
Predict LCA for the entire life cycle



Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

End-of-Life of lubricants (here base oils)

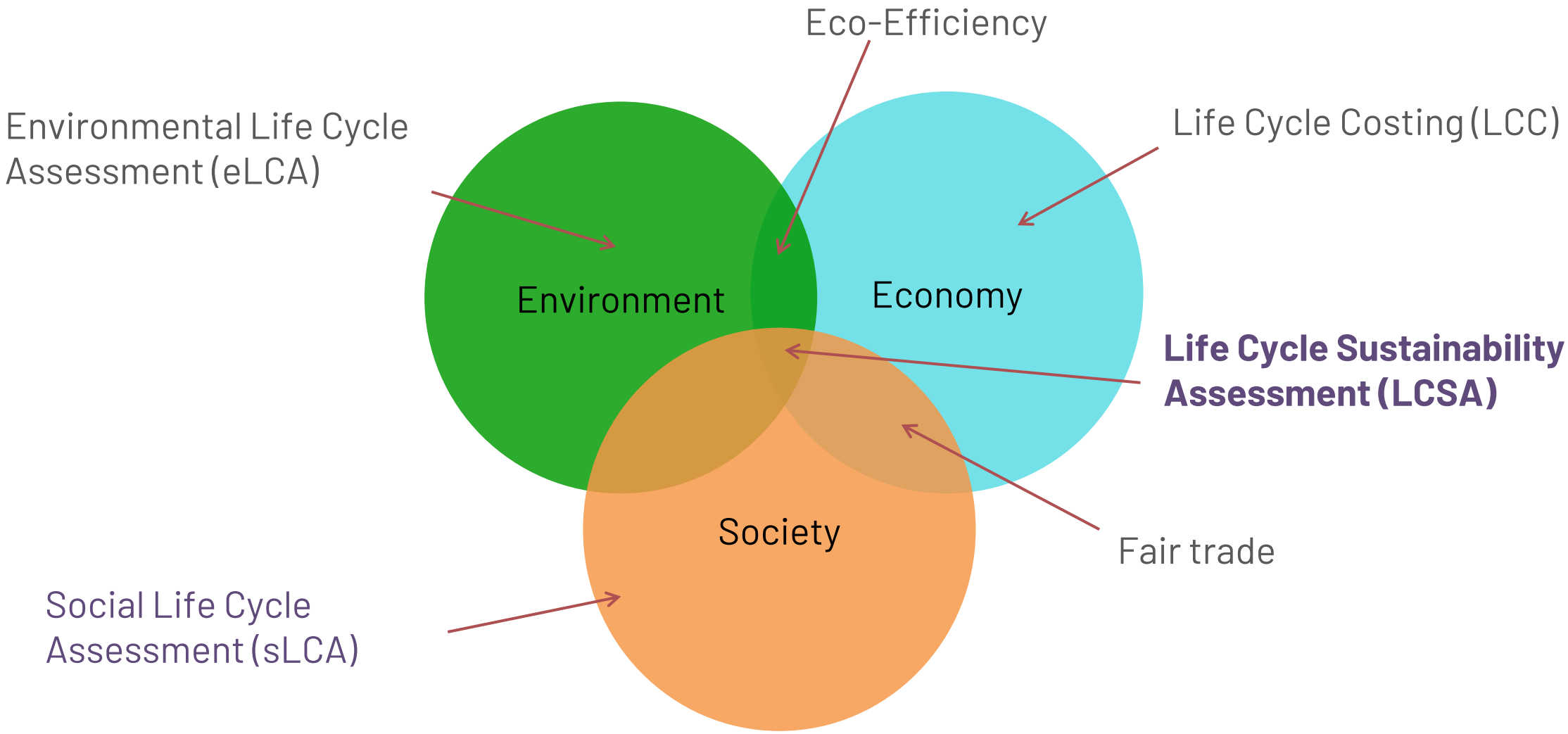


Used Oil Management and Beneficial Reuse Options to Address Section 1: Energy Savings from Lubricating Oil Public Law 115-345, Report to Congress, ***2020****, Washington.*

Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

More than LCA → life cycle sustainability assessment



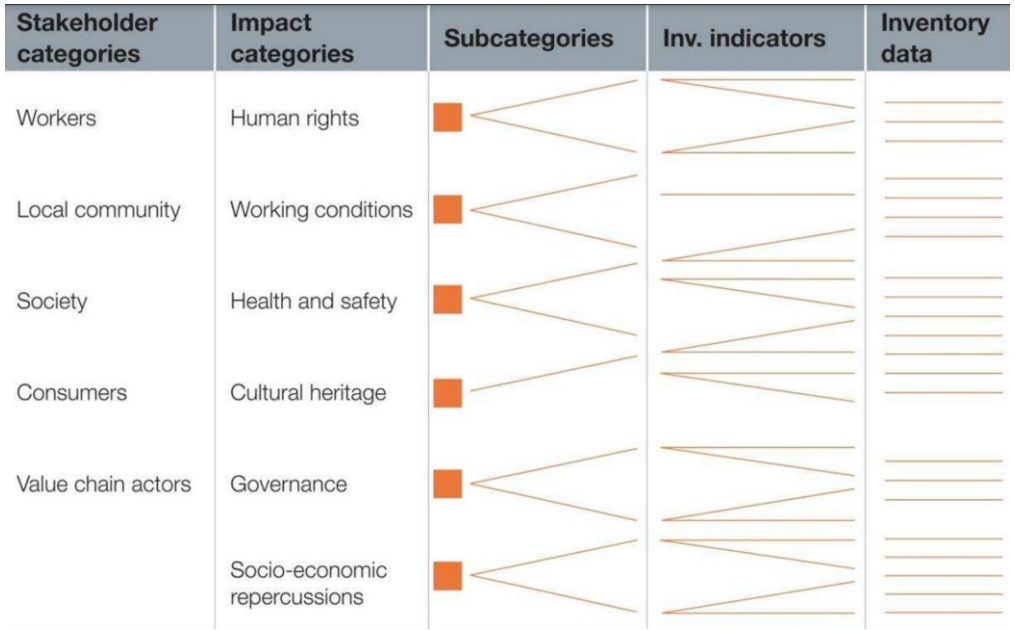
Socioeconomic assessment (SSbD)

Economic dimension:

- **Life Cycle Costing (LCC)**
  - Compares cost across life cycle
  - including **internal** (materials, labour, energy) and **societal** costs (environmental and social externalities)
- **Criticality Assessment (CRM)**
  - Flags presence of **CRM**s in supply chain
  - Lithium, cobalt and rare earth elements

Social dimension:

- **Social LCA is a technique to assesses social/socio-economic aspects and impacts**
- **Various stakeholder and social indicators**



- **Data can be derived from databases (PSILCA)**

Conclusion

- SSbD is a **voluntary pre-market** approach developed by the JRC
- It focuses on **safety, environmental and socioeconomic** dimensions
  - All chemical innovations should be safe than sustainable
- To assess the sustainability, the **whole life cycle** has to be assessed
  - This is in particular important for lubricants (Use/EoL phase)
- By **simulating the whole SSbD cycle**, time/money can be saved
  - Please consider following our research project SiToLub
- Feel free to talk with me about LCA and SSbD. Let's discuss!

Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

Thank you!

Jonas Hoffmann
GreenDelta GmbH
hoffmann@greendelta.com

Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

Annex
Simulation Example

Jonas Hoffmann
GreenDelta GmbH
hoffmann@greendelta.com

Co-funded by the European Union

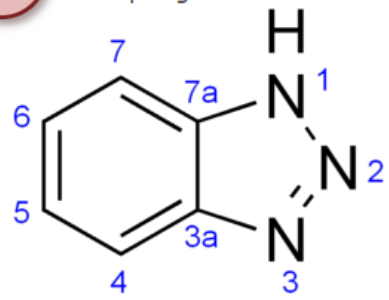
Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

WORKING FLOW

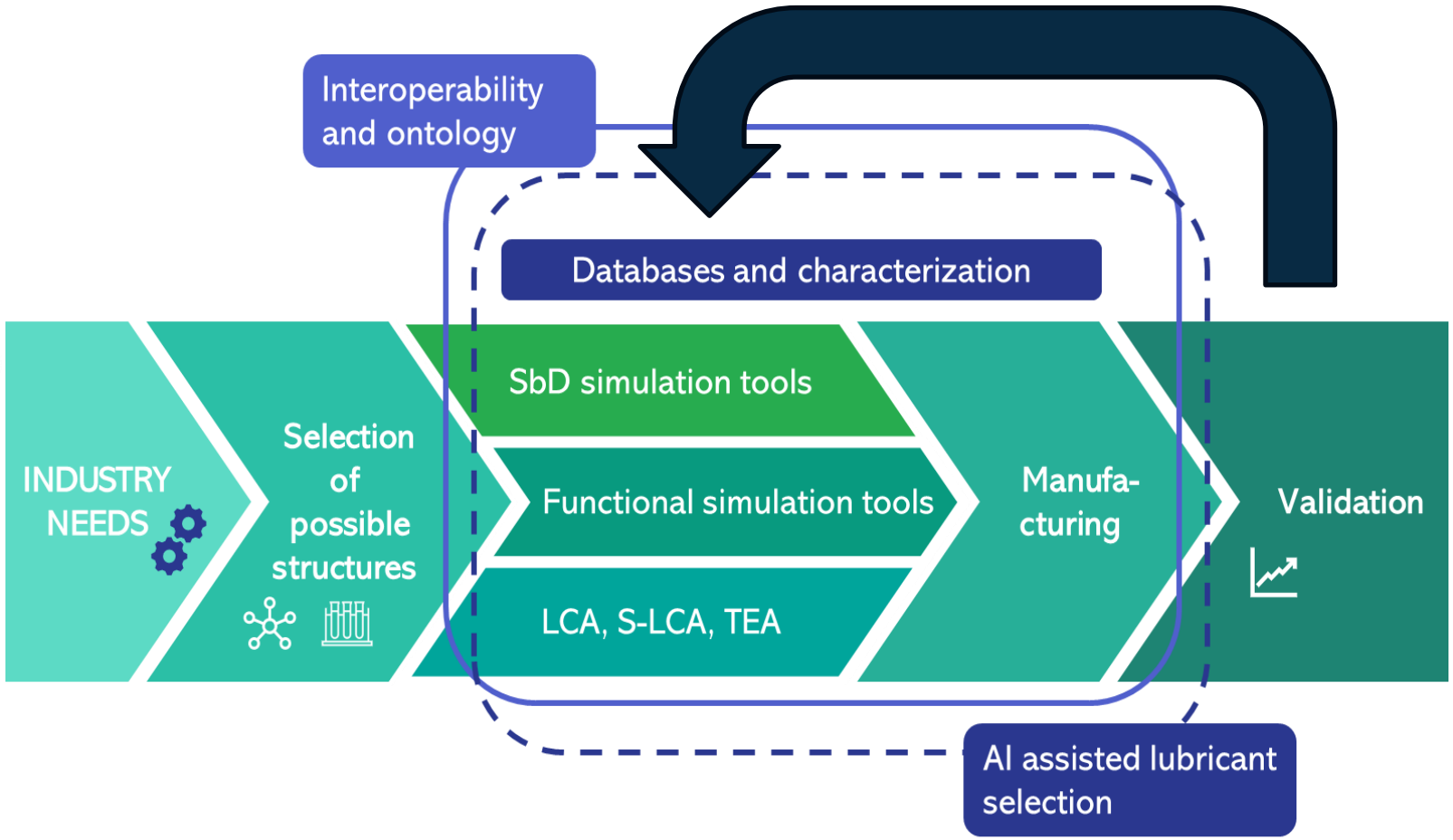
Properties of concern

PBT Under assessment as Persistent, Bioaccumulative and Toxic

ED Under assessment as Endocrine Disrupting



benzotriazole

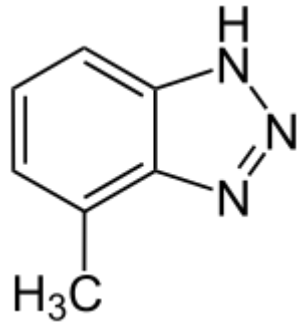


Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

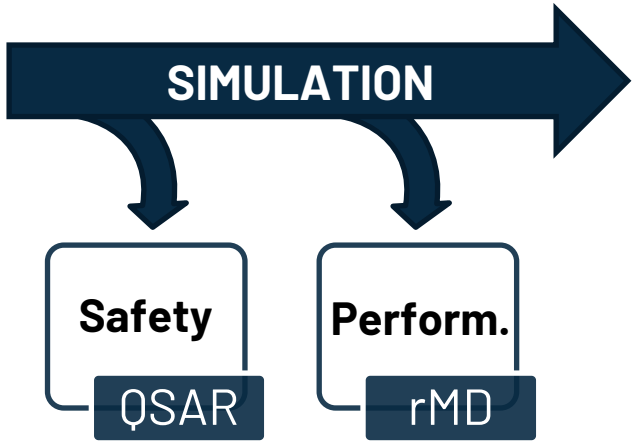
The Challenge:
Predict LCA for the entire life cycle

Platform – Input

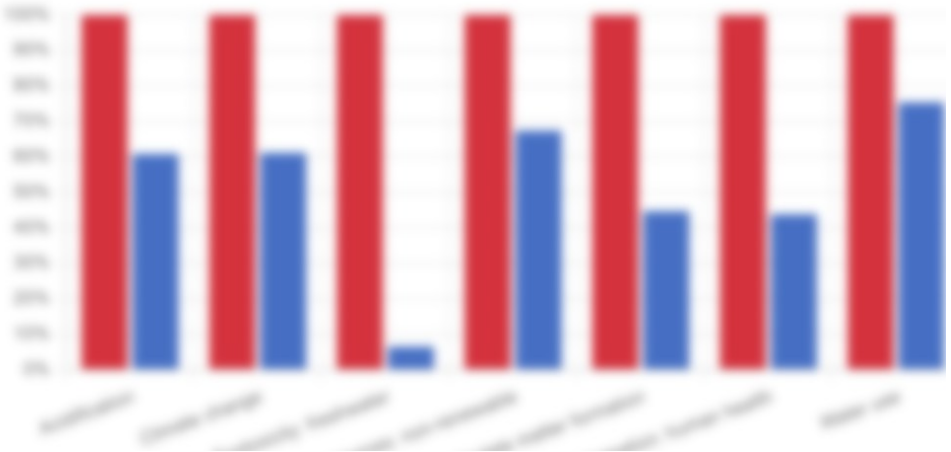


n1c2ccccc2[nH]n1

SMILES CODE
(or CAS)



Platform – Output

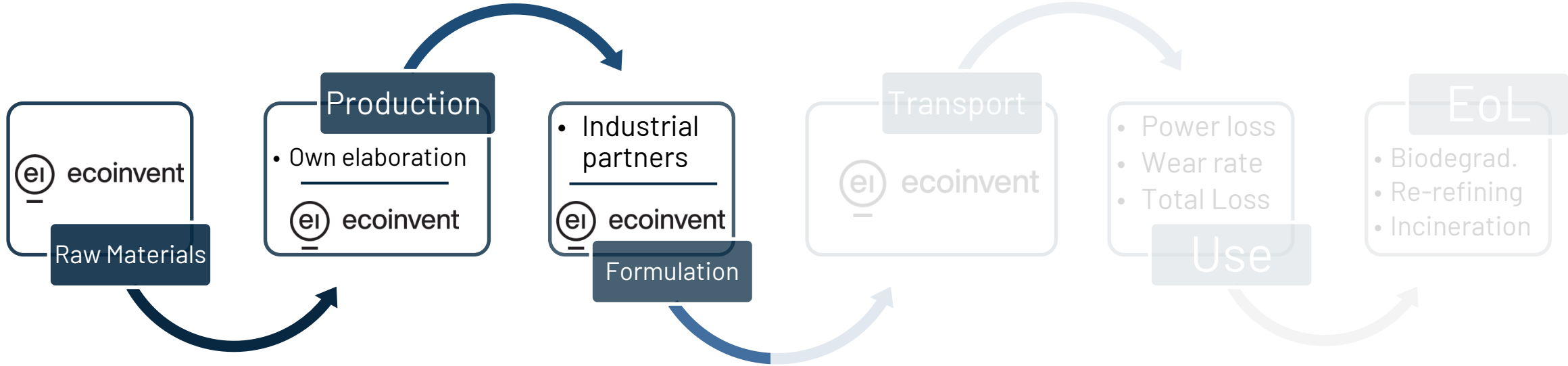


ENVIRONMENTAL IMPACTS
Cradle-to-Grave

Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

The Challenge:
Predict LCA for the entire life cycle



Impacts (rule of thumb)

33%

66%

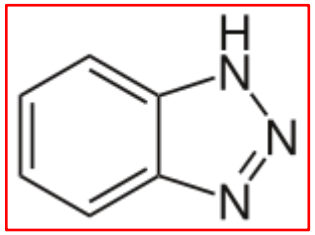
SSbD base case

SSbD alternative

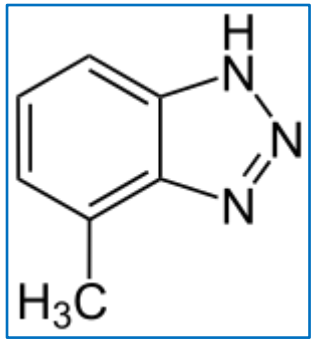
Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

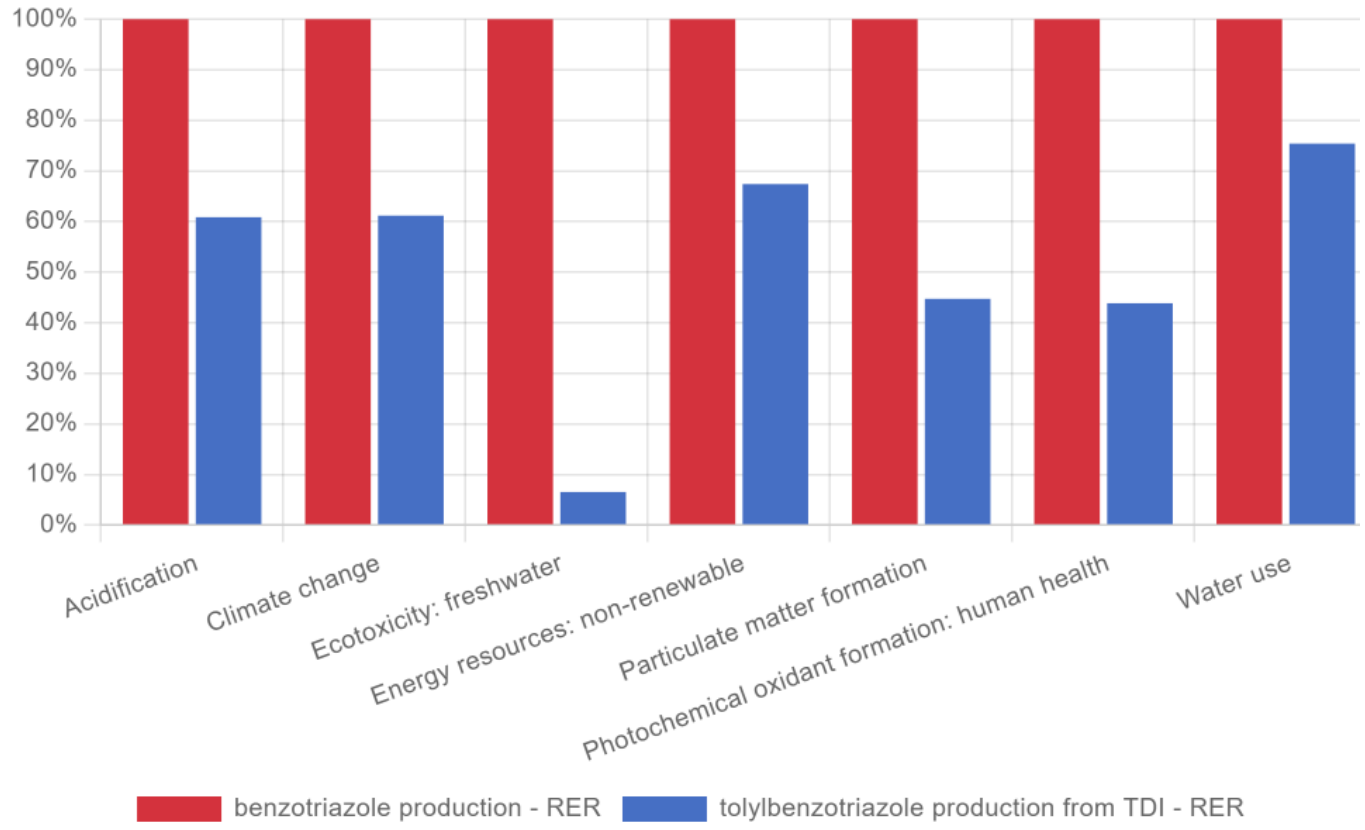
Raw Material Extraction and Production: The case of tolyltriazole (cradle-to-gate)



SSbD base case



SSbD alternative



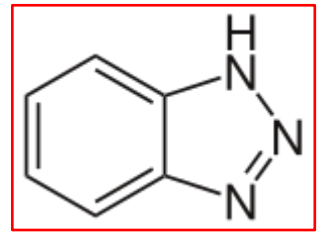
cradle-to-gate, referenced to 1 mol of product, ecoinvent 3.11, EF 3.1 LCIA

Co-funded by the European Union

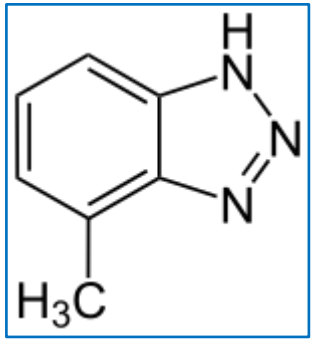
Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

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

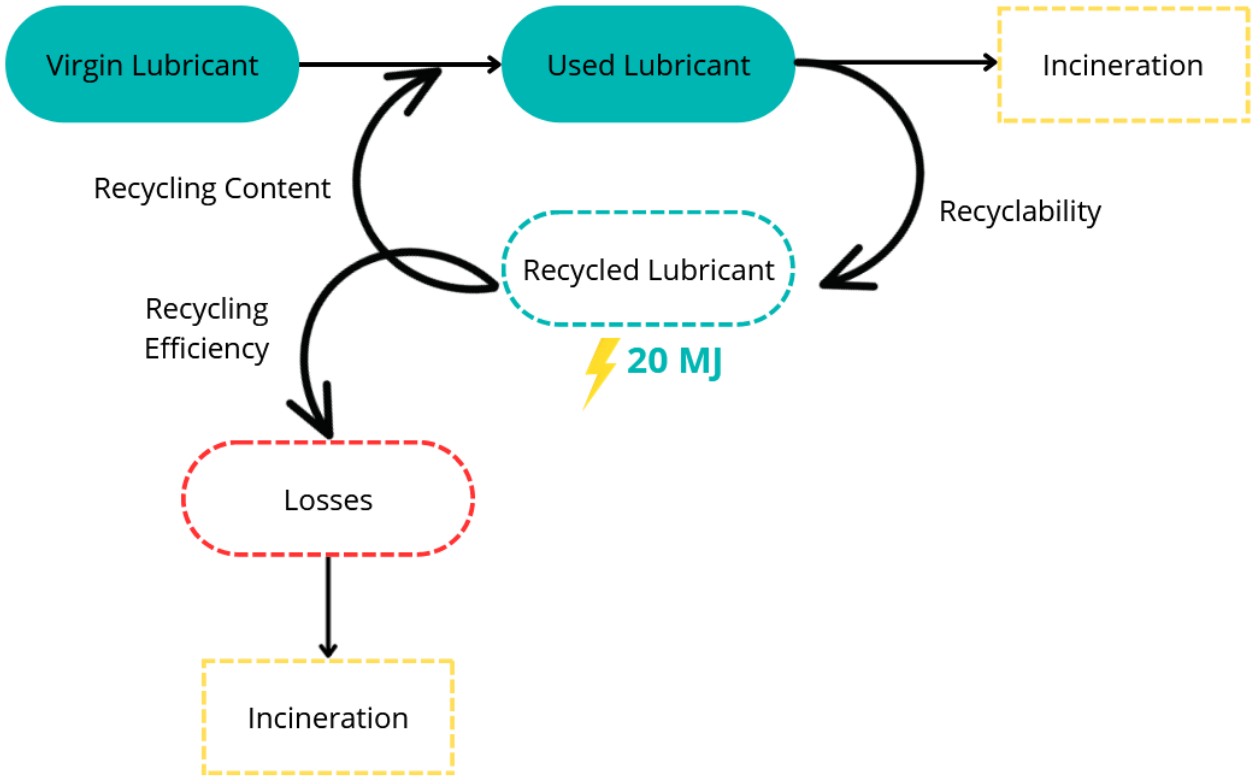
Future development:

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

Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

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)

Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

SSbD scoring

Evaluation system

Position to target	Score	Color code	
>Target + 50%	0		Fail the criteria
>Target; <Target + 50%	1		
>Target - 25%; **<Target**	2		Pass the criteria
>Target - 50%; <Target -25%	3		
<Target – 50%	4		

Example of a summary table of the evaluation of step 4

LCA Assessment level	Aspect	Score
Toxicity	Human Toxicity cancer	3
	Human Toxicity non cancer	2
	Ecotoxicity	1
Climate Change	Climate Change	3
Pollution	Ozone depletion	4
	Particulate matter/Respiratory inorganics	2
	Ionising radiation, human health	2
	Photochemical ozone formation	1
	Acidification	0
	Eutrophication, terrestrial	4
	Eutrophication, aquatic freshwater	3
	Eutrophication, aquatic marine	2
Resources	Land Use	4
	Water use	2
	Resource use, minerals and metals	2
	Resource use, energy carriers	2

Co-funded by the European Union

Co-Funded by the European Union under the Grant Agreement No. 101138807. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.