GreenDelta
sustainability consulting + software

openLCA

# Life Cycle Assessment as Key Element of Safe and Sustainable by Design Lubricants

Picture: Julia Cilleruelo Palomero

Dr. Jonas Hoffmann, GreenDelta GmbH, Berlin
on 18 February, 2026, organized at Punjab Engineering College

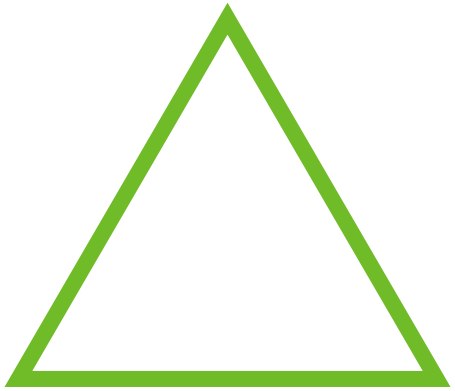
# GreenDelta background

- Founded by Dr. Andreas Ciroth in 2004, Berlin
- ~ 25 employees (engineers, biologists, IT specialists, business admin., chemist)
- Business world-wide: sustainability research, life cycle assessments, databases, software for life cycle assessments and sustainability

# GreenDelta, What we do

Sustainability consultancy and research

environmental LCAs, resource criticality, social LCAs, LCC



Database development and distribution

Software development, especially open source

# Software: openLCA

- World's leading open source tool for LCA and sustainability assessment. Powerful, free, developed since 2006 by GreenDelta.
- Open-source under mozilla license (transparent via github)
- Supported by US EPA, USDA, JRC, ...
- Widest selection of databases, including ecoinvent

# Data: Nexus

- World's largest repository of LCA databases: IO Databases, product-based databases, libraries, for openLCA, some for SimaPro, developed and operated by GreenDelta since 2014
- Databases prepared by GreenDelta
- > 150,000 datasets, all major LCA databases, > 30,000 users
- https://nexus.openlca.org/

# Projects: My tasks as sustainability consultant

Software trainings for openLCA, Research proposals
Database management (**Environmental Footprint 3.1 by JRC**)

PRIMUS

Holistic sustainability assessment of plastic recyclates

KIETA

Software-solutions for heat distribution (steam) in communes

TriFluorium
safe fluorine circularity

Ecologic/Economic assessment of AI-supported plastic recycling

SiToLub

Simulation of life cycle sustainability assessments with SSbD lubricants



*see also https://www.greendelta.com/projects/*

SiToLub

SIMULATION TOOLS FOR THE DESIGN OF
**SAFE AND SUSTAINABLE LUBRICANTS**

# Predictive Sustainability Assessment of Novel SSbD-Lubricants


This project has received funding from the European Union's **Horizon Europe** research and innovation programme (innovation action) under grant agreement No. 101138807

**Defintion**: A substance that is introduced between two surfaces and change their interaction, mainly by reducing the friction needed for sliding or reducing the wear generated during the relative movement.

**Function**:

- Reducing friction between moving parts
- Removing heat from working parts
- Cleaning and sealing surfaces of machine parts
- Extends lifespan and reduces energy losses (exergy)

**Lubricants contribute to sustainability!**

# APPLICATIONS FOR LUBRICANTS

**Consideration**:

- Essential for transport and e-mobility
- Required for green energy technologies (wind mills, steam..)
- Essential for recycling of materials
- With improved lubricants 1460 Mt $CO_2$/y and 1.4% of global GDP can be saved[1]

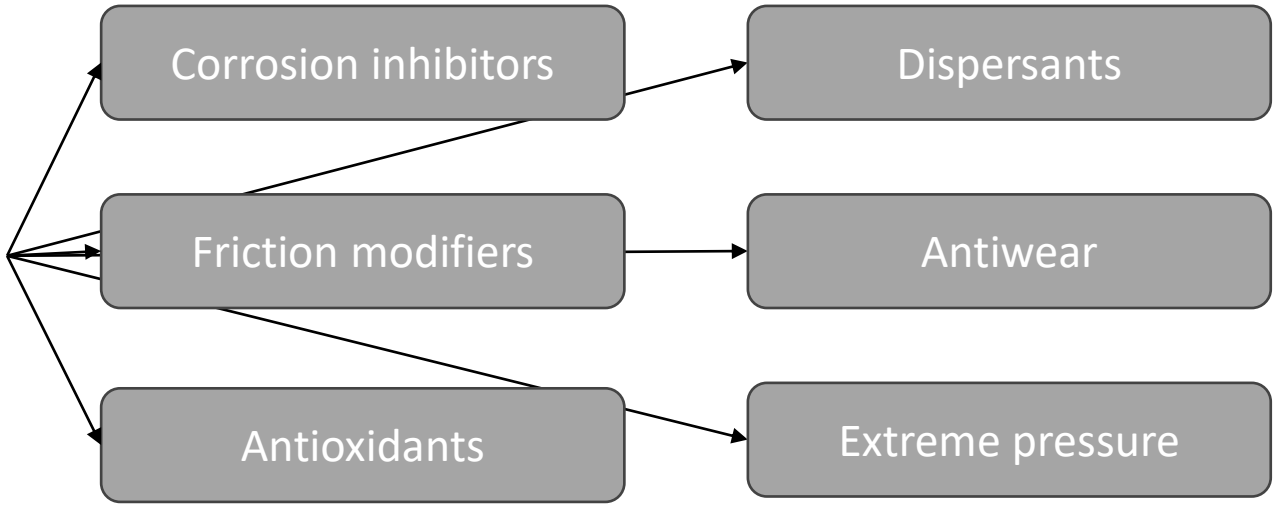





[1] K. Holmberg, A. Erdemir, *Friction* **2017**, 5, 263–284.

# Lubricant formulation:

| | 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 | | | |



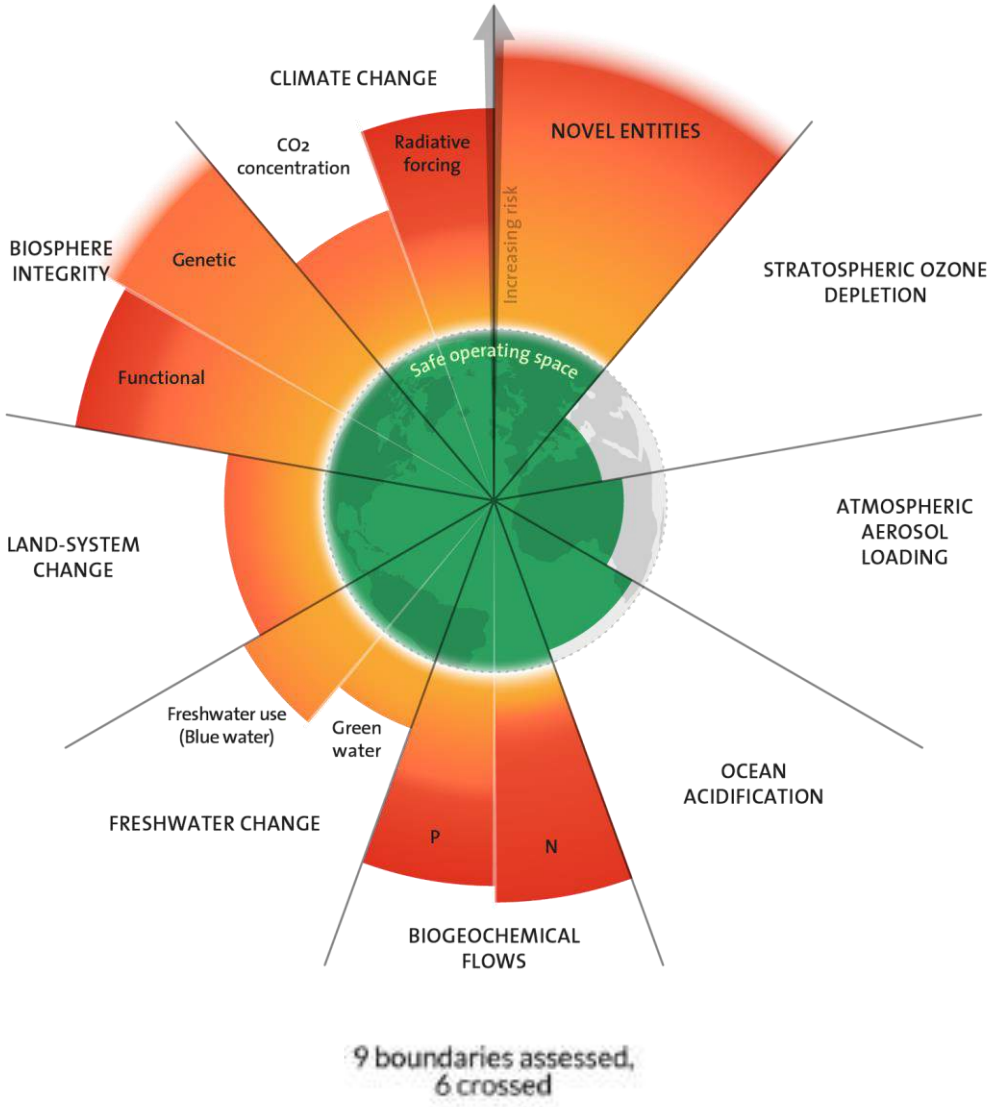

## What industry is facing:


## What costumers want:




## Industry is in need for novel safe and sustainable solutions!

# Planetary Boundaries

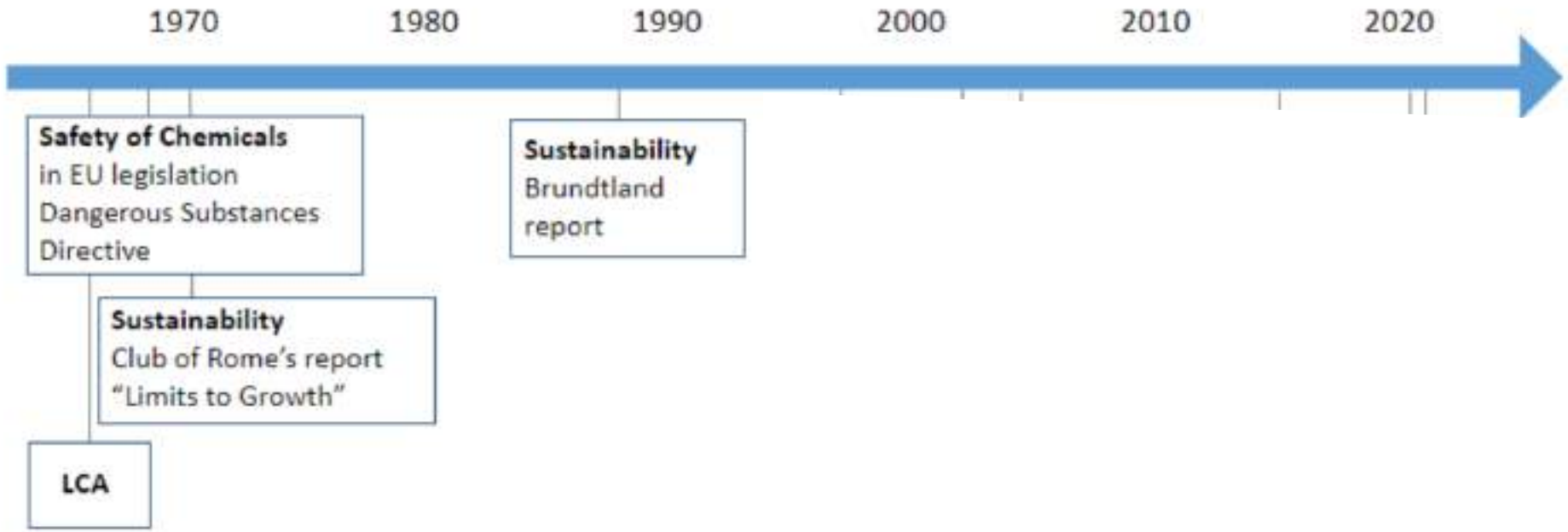



*'With such an enormous percentage of untested chemicals being released to the environment,* ***a novel entities boundary*** *defined in this manner is* ***clearly breached****.'*



Rockström *et al*., *Sci. Adv.* **2023**, 9, DOI 10.1126/sciadv.adh2458.

# Sustainability within the Chemical Industry



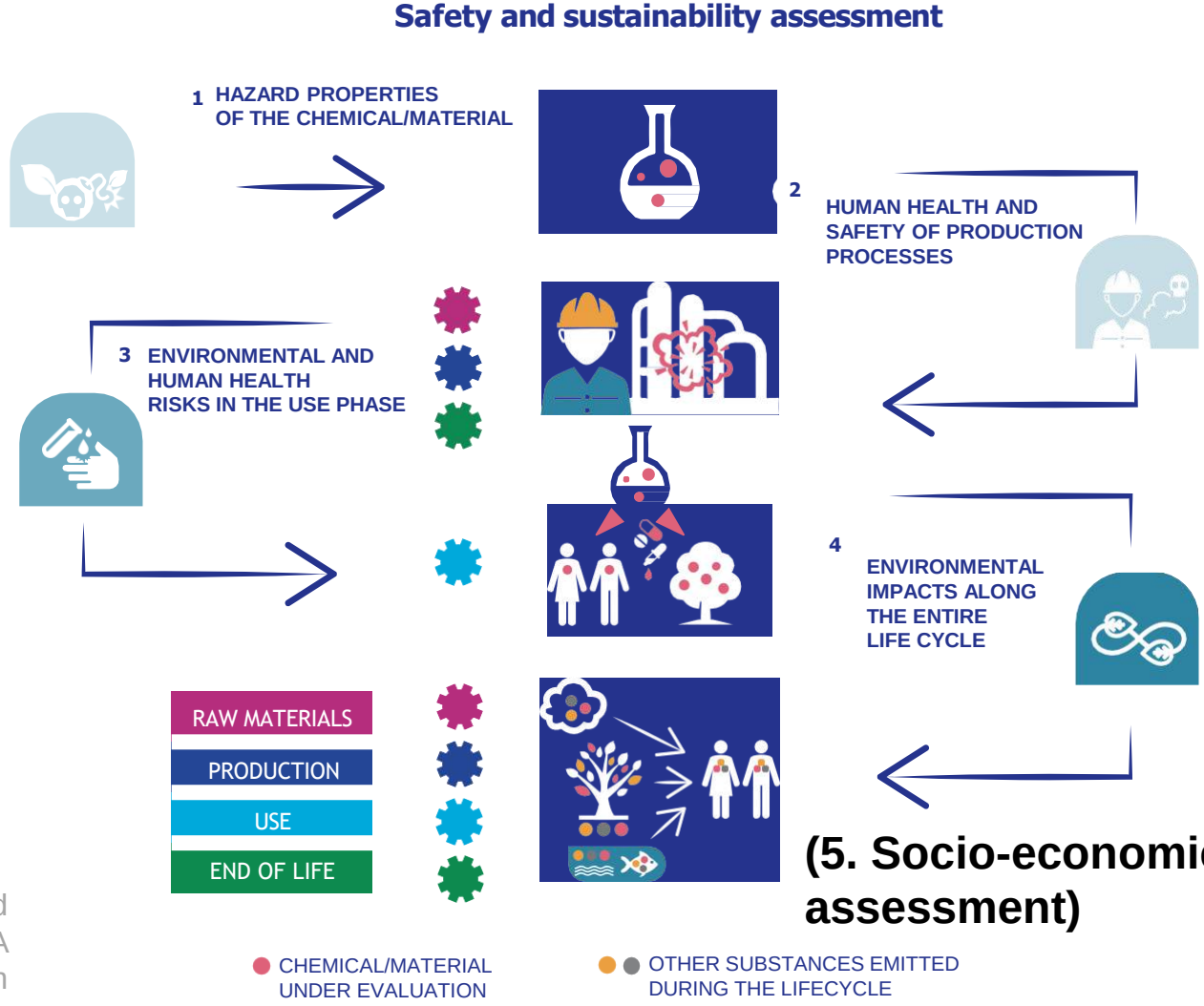

*'The SSbD framework promotes such a **holistic approach** that integrates **safety and sustainability** of chemicals, materials, products and processes throughout their **entire life cycle** and **minimizes** their **environmental footprint**.'*

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

# 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

# Safe and Sustainable by Design – Design Criteria

| Code | SSbD principle | Indicator | Best case | Worst case |
|---|---|---|---|---|
| SSbD1 | Material efficiency | Net mass of materials consumed (kg/kg) | 1 | 40% |
| | | Reaction Yield (%) | 100% | 40% |
| | | Atom Economy (MWproduct/MWtotal reaction) | 100% | |
| | | Material Intensity index (kg materials / kg product) | 100% | |
| | | Environmental impact factor - E-factor (%) (Input materials - product)/product | 0% | |
| | | Recycling of the solvent and purity | 99 -100% (purity) | |
| | | Solvent selectivity (kgsolvent/kgproduct) | 0% | |
| | | Water consumption ($m^3$/kg) | 0 | 2.95 |
| | | Recycling efficiency/recovery rate (%) | 100% | |
| | | Total amount of waste (kg/kg) | 0% | |
| | | Amount of waste to landfill (kg/kg) | 0% | 100% |
| | | Critical Raw Material presence (yes/no + amount) | 0% | 100% |
| SSbD2 | Minimise the use of hazardous chemicals/materials | Biodegradability of manufactured chemical/Material | 100% | 0% |
| | | Classification of raw chemicals/materials as SVHC (yes/no + amount) | 0% | 1 kg/kg |
| SSbD3 | Design for energy efficiency | Energy efficiency (%) | Min theoretical energy ΔG kJ/kg | 1.949x10^6 kJ/kg |
| | | Yield of extraction (mass of recovered solvent / used solvent) | 100% | 0% |

| Code | SSbD principle | Indicator | Best case | Worst case |
|---|---|---|---|---|
| SSbD4 | Use renewable sources | Renewable or fossil feedstock (yes/no + amount) | 100% | 0% |
| | | Recycled content (%) | 100% | 0% |
| | | Share of Renewable Energy (%) | 100% | 0% |
| SSbD5 | Prevent and avoid hazardous emissions | Non-Aqueous Liquid Discharge ($m^3$/kg) | 0% | 100% |
| | | Wastewater to treatment ($m^3$/kg) | 0% | 100% |
| | | Amount of hazardous waste (kg/kg) | 0% | 1 kg/kg |
| SSbD6 | Reduce exposure to hazardous substances | Biodegradability of manufactured chemical/Material | 100% | 0% |
| | | Classification of raw chemicals/materials as SVHC (yes/no) | 0% | 100% |
| SSbD7 | Design for end-of-life | Recyclable? (yes/no) | 100% | 0% |
| | | Durability (years) | | 0-1 |
| | | Disassembly/reparability design (yes/no) | 100% | 0 |
| SSbD8 | Consider the whole life cycle | Recyclable? (yes/no) | 100% | 0% |
| | | Disassembly/reparability design (yes/no) | 100% | 0% |
| | | Material Circularity indicator (MCI) | 1 | 0 |
| | | Biodegradability of manufactured chemical/Material | 100% | 0% |

# SSbD – 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!**

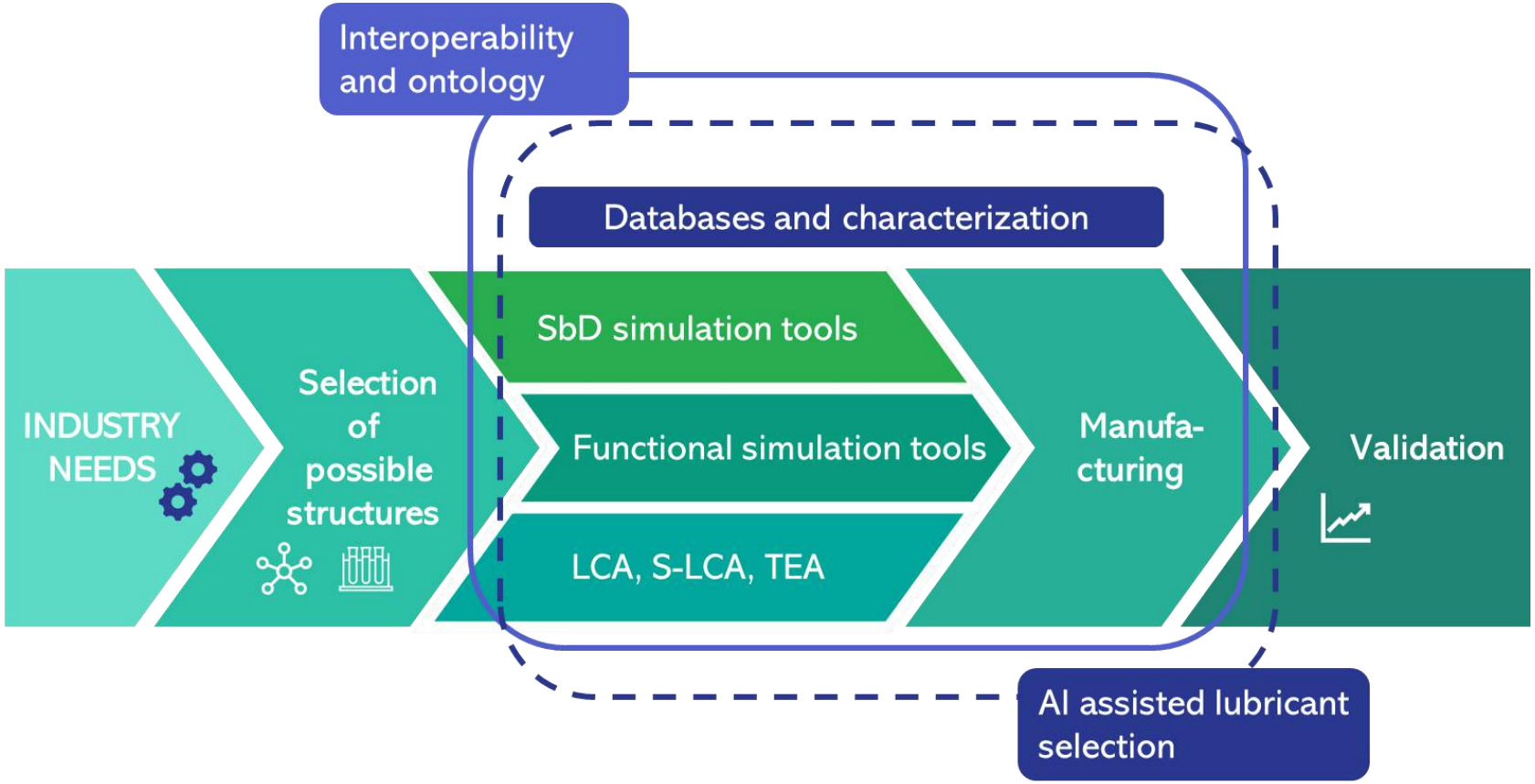
Caldeira, C., Garmendia Aguirre, I., Tosches, D., Mancini, L., Abbate, E., Farcal, R., Lipsa, D., Rasmussen, K., Rauscher, H., Riego Sintes, J. and Sala, S., Safe and Sustainable by Design chemicals and materials - Application of the SSbD framework to case studies, Publications Office of the European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

**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

# SiToLub - WORKFLOW




# Simulation Approach in SiToLub

ProtoQSAR
Computational toxicology: fast, economical and ethical

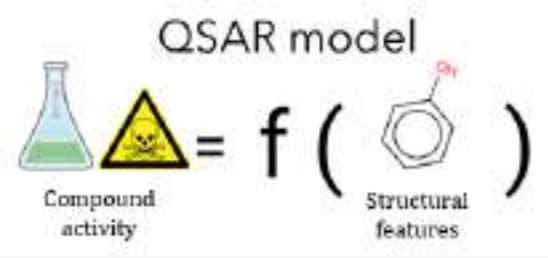
## QSAR Simulation

Quantitative

Structural

Activity

Relationships



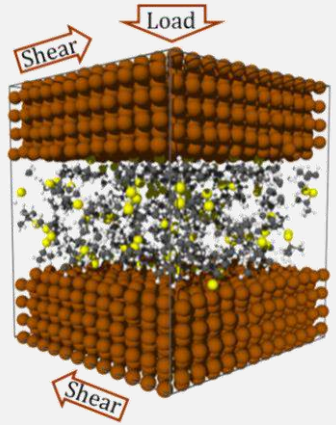

**(Eco)Tox. & Biodegr.**

ACT research

## Performance Sim.

- Evaluation for lubricants and their components

- Reactive MD simulation

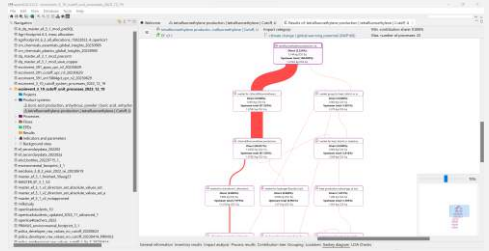



**Performance**

GreenDelta

## Sustainability Sim.

- Environmental Impacts
- Social Impacts
- Economical Impacts



**Sustainability**

# Safe and Sustainable by Design

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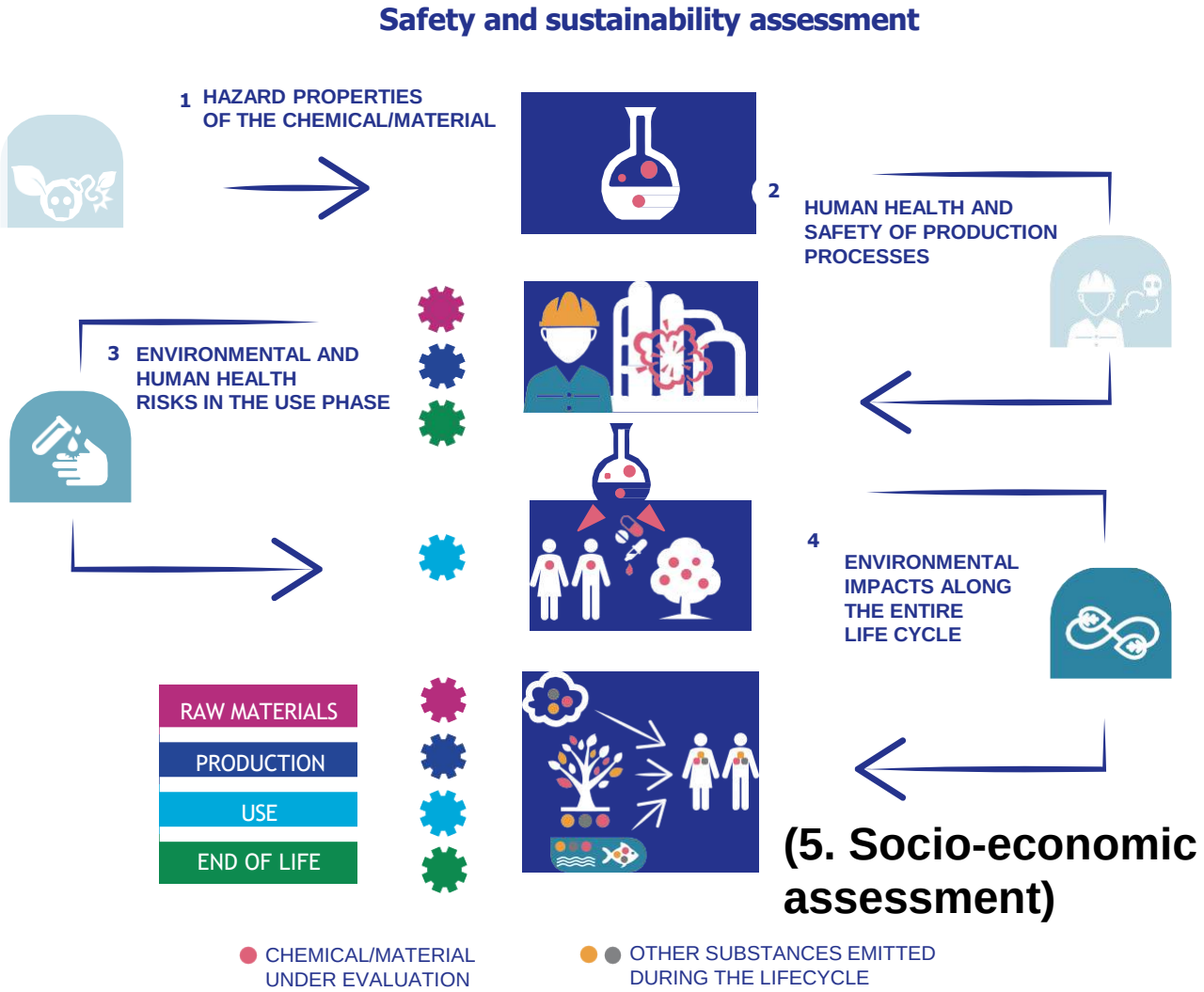



European Commission, Directorate-General for Research and Innovation, Safe and sustainable by design chemicals and materials – A European assessment framework, Publications Office of the European Union, 2022, https://data.europa.eu/doi/10.2777/86120

# 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.'*

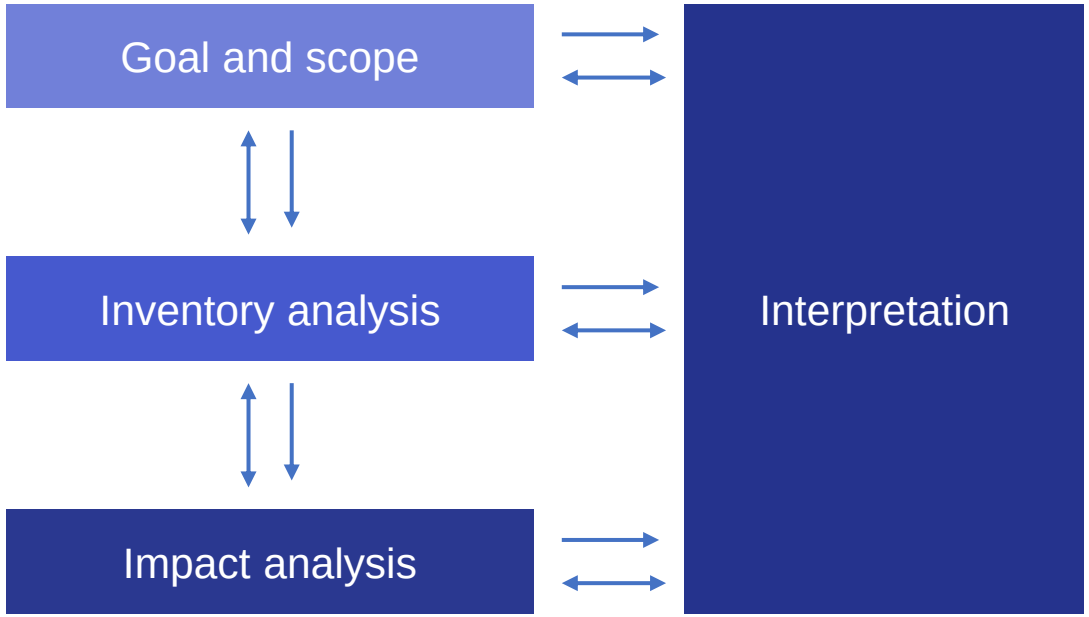



European Commission, Joint Research Centre, Cristobal-Garcia, J., Pant, R., Reale, F. et al., Life cycle assessment for the impact assessment of policies, Publications Office, 2016, https://data.europa.eu/doi/10.2788/318544

# Life Cycle Assessment: Structure

- LCA approach is mainly based on two standards: **ISO 14040:2006 and ISO 14044:2006**
- LCA is performed in **four steps:**
  1. Goal and Scope definition
  2. Life Cycle Inventory
  3. Life Cycle Impact Analysis
  4. Life Cycle Interpretation
- Most important concept in LCA: **Functional Unit**

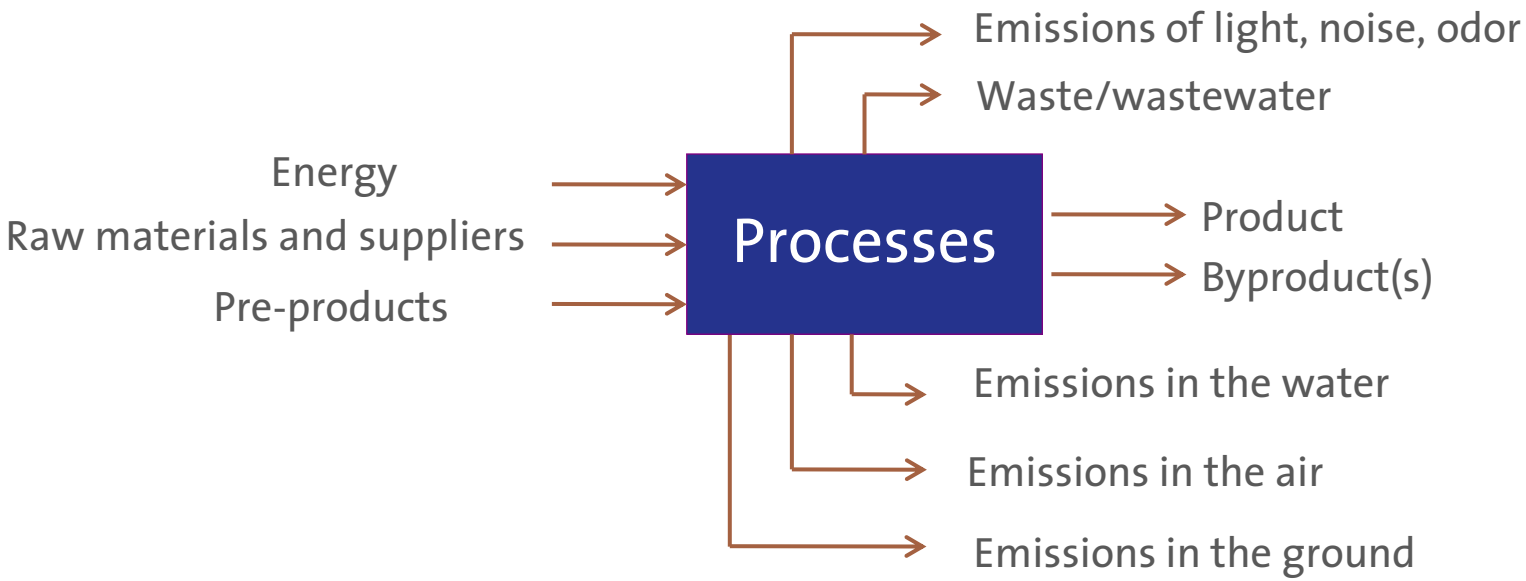
**Life Cycle Assessment framework**



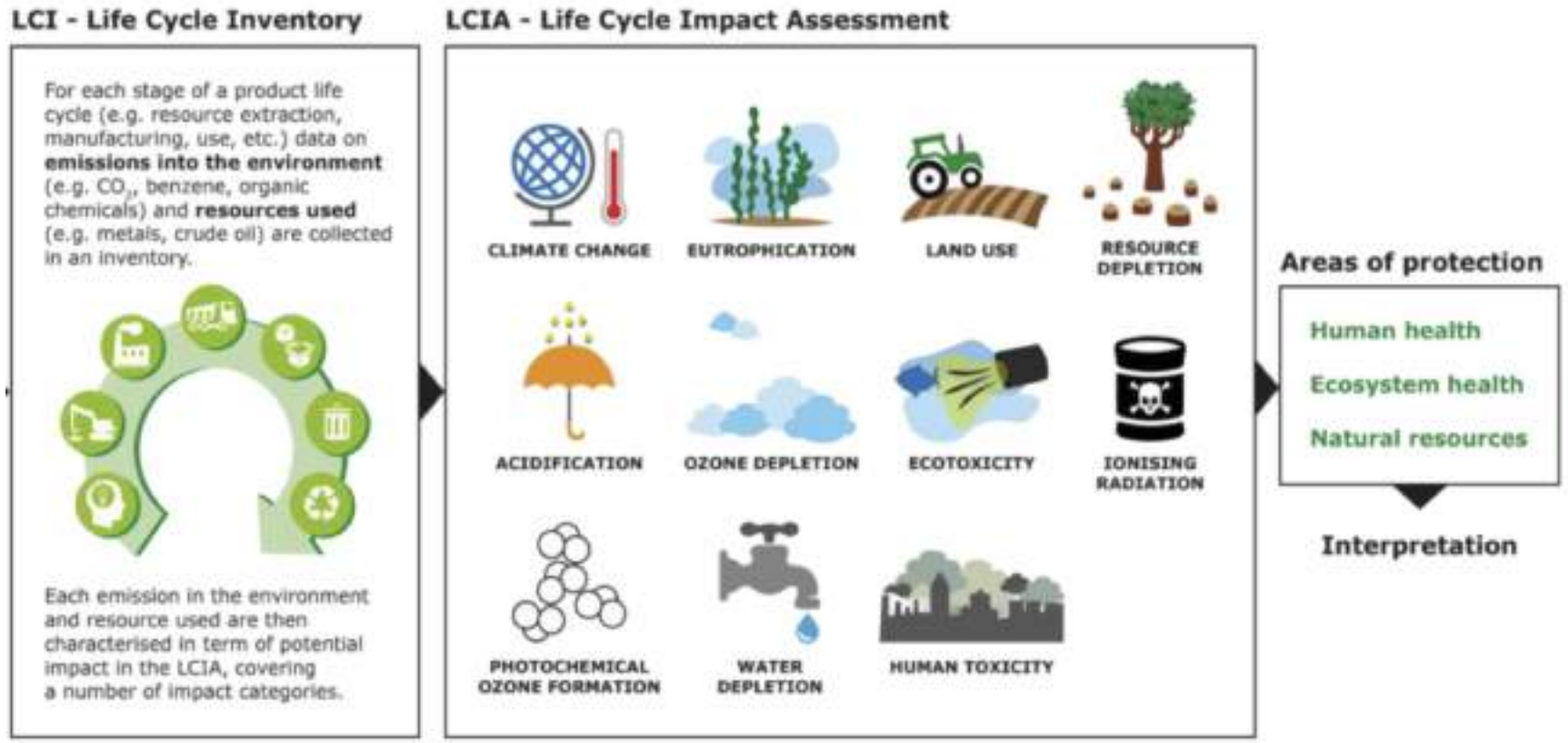

**Functional Unit Definition**: 'quantified performance of a product system for use as a reference unit': Examples: 100 calories of food, 1 person*km, x produced parts by using x kg of lubricant

# Life Cycle Inventory – Data needed

## Inputs and outputs of a process to be included in the LCI



# Life Cycle Inventory, Impact Assessment and Interpretation




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

# **SITOLUB** – Use Cases

1. Metal-cutting lubricants (chl. paraffins)
2. PFAS-based lubricants
3. Corrosion inhibitors

## Life Cycle Assessment: Structure

LCA approach is mainly based on two standards: **ISO 14040:2006 and ISO 14044:2006**
LCA is performed in **four steps:**

1. Goal and Scope definition
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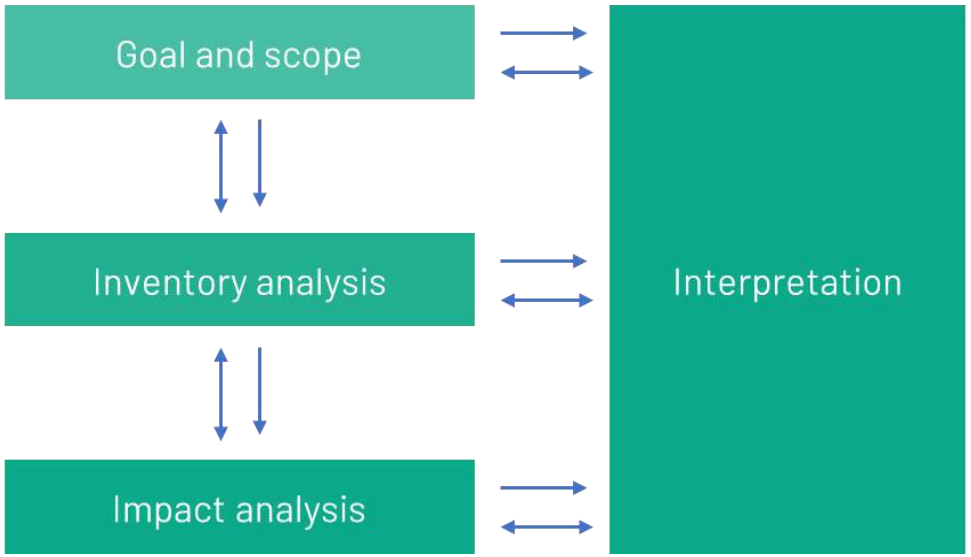
3. Life Cycle Impact Analysis
4. Life Cycle Interpretation

**Life Cycle Assessment framework**

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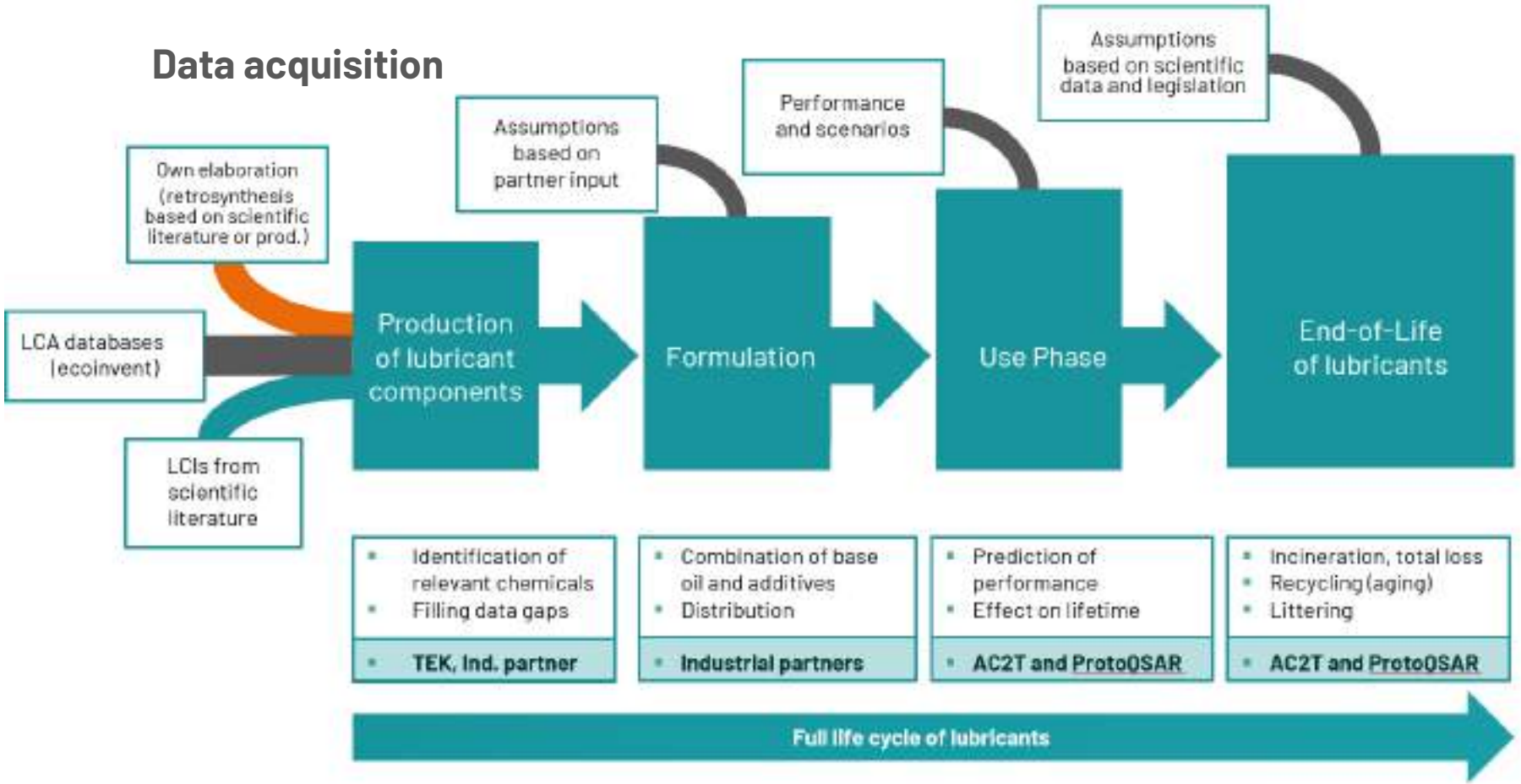
## Data acquisition for Sustainability models




Various sources for LCIs and assumptions

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

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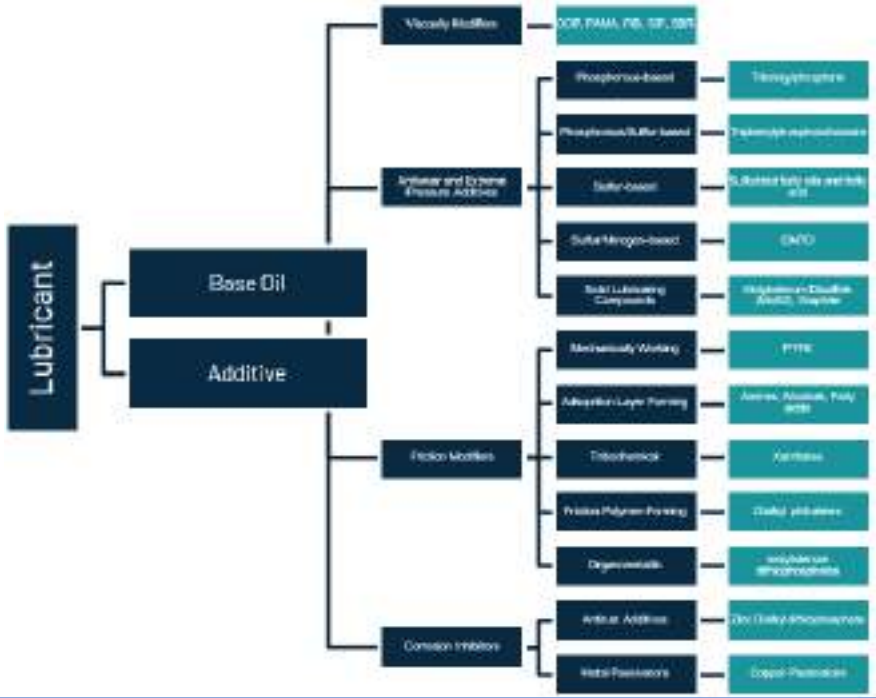
# Life Cycle Assessment (LCA) of lubricant components

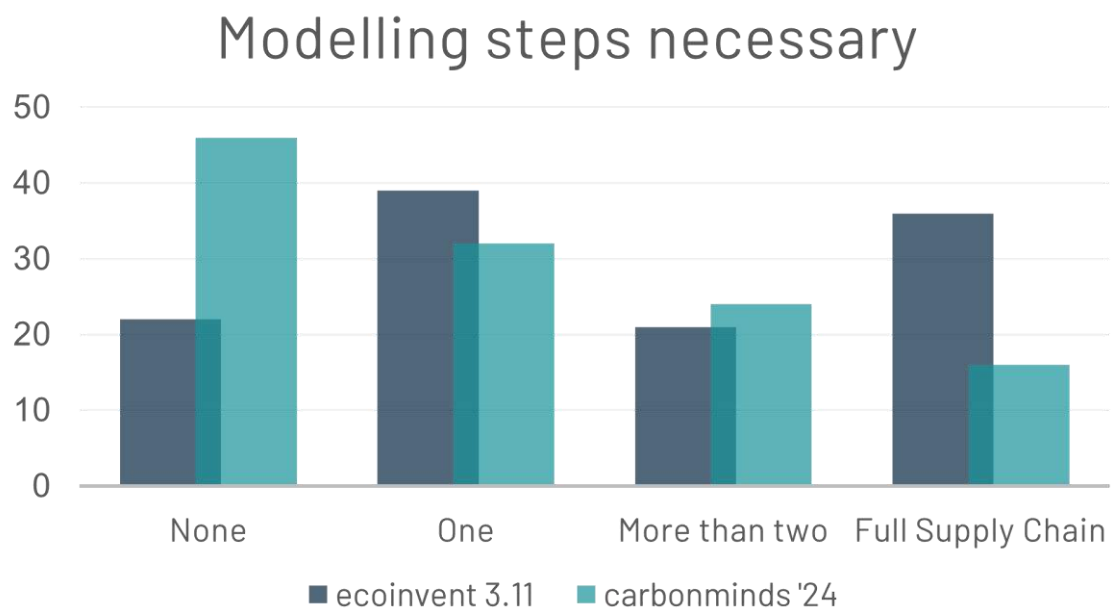
## Data acquisition for Sustainability models

### Data categorisation (150 chemicals)




Users can select the SSbD base case or the formulation

### Selection of background database




While CarbonMinds is more suitable for lubricants but lacks general processes, e.g. transport, EoL etc.; ecoinvent will be the background

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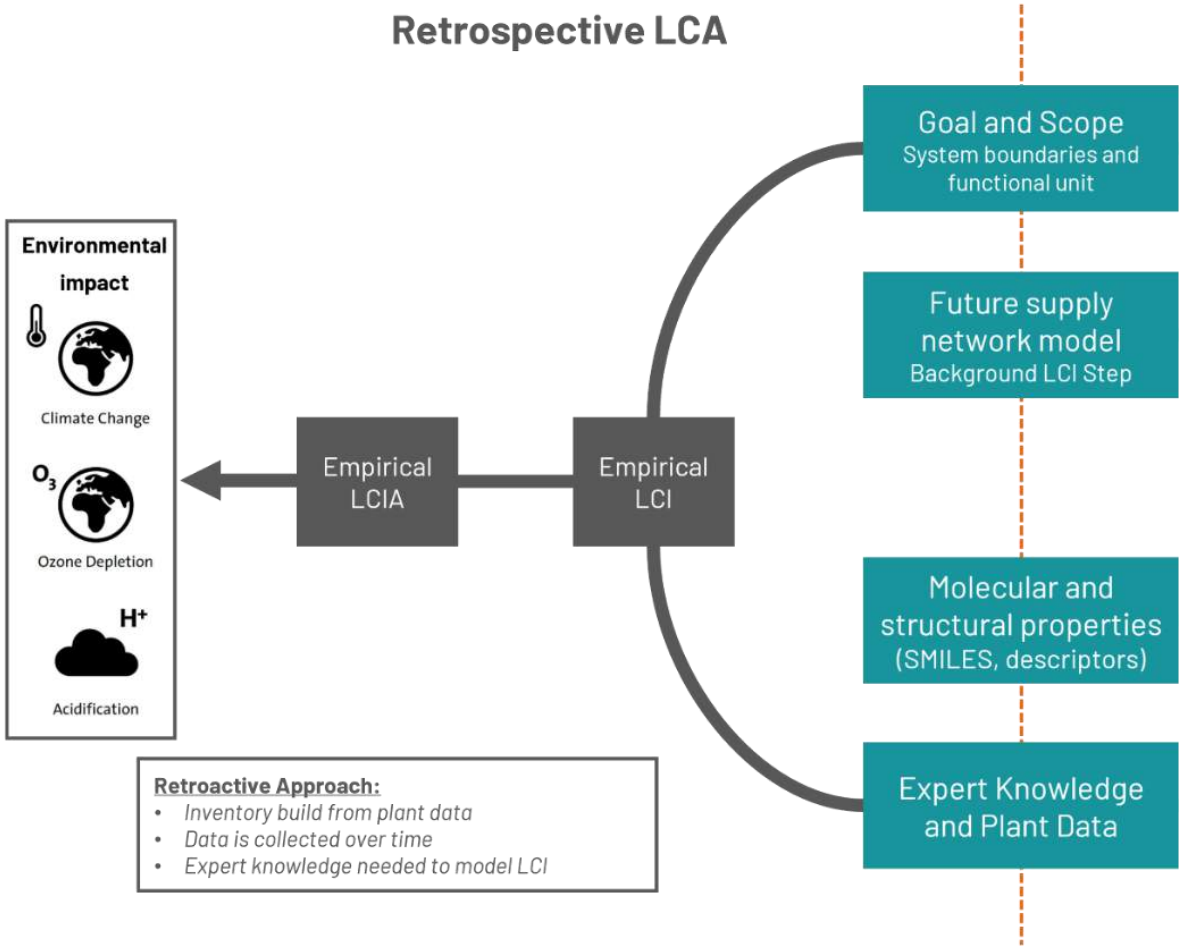
## How to fill data gaps (production)

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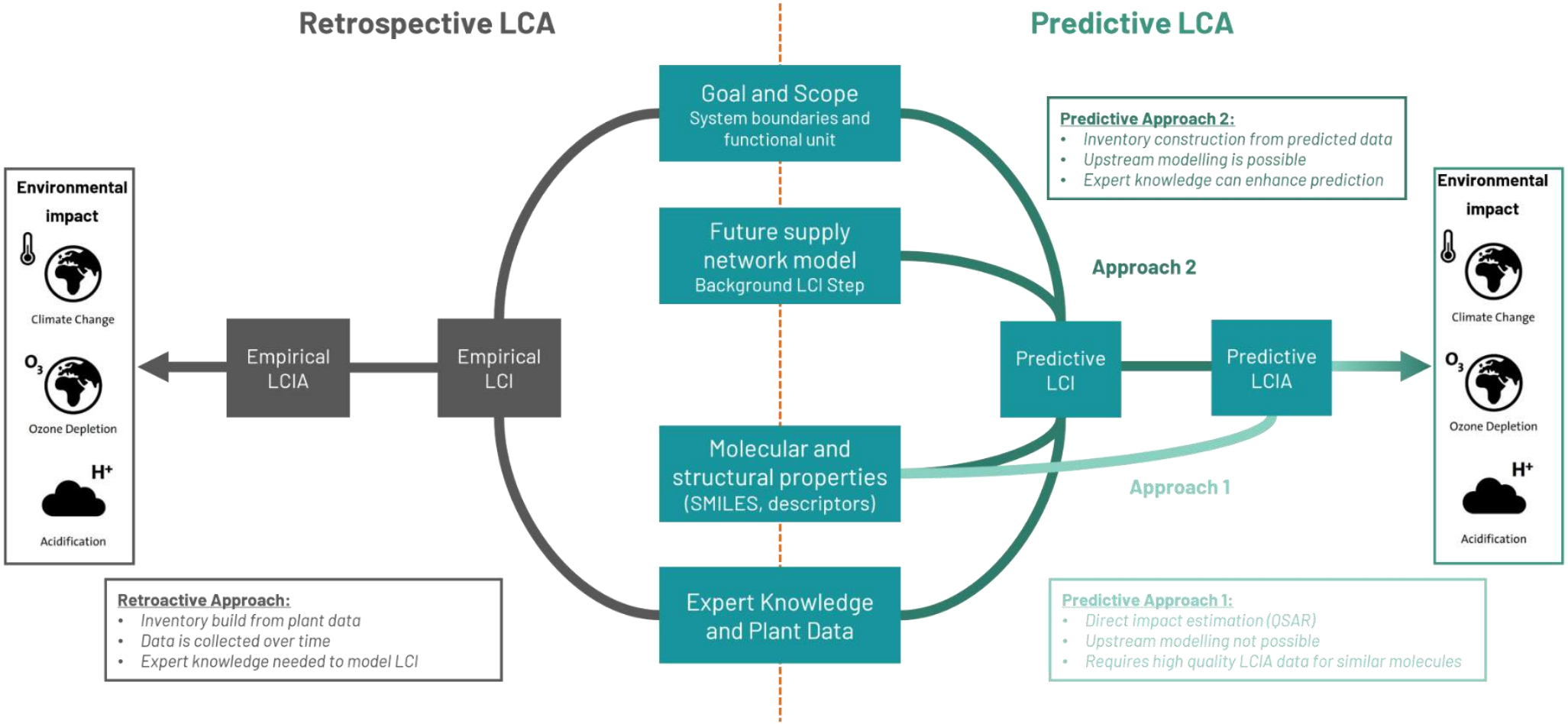
## How to fill data gaps (production)

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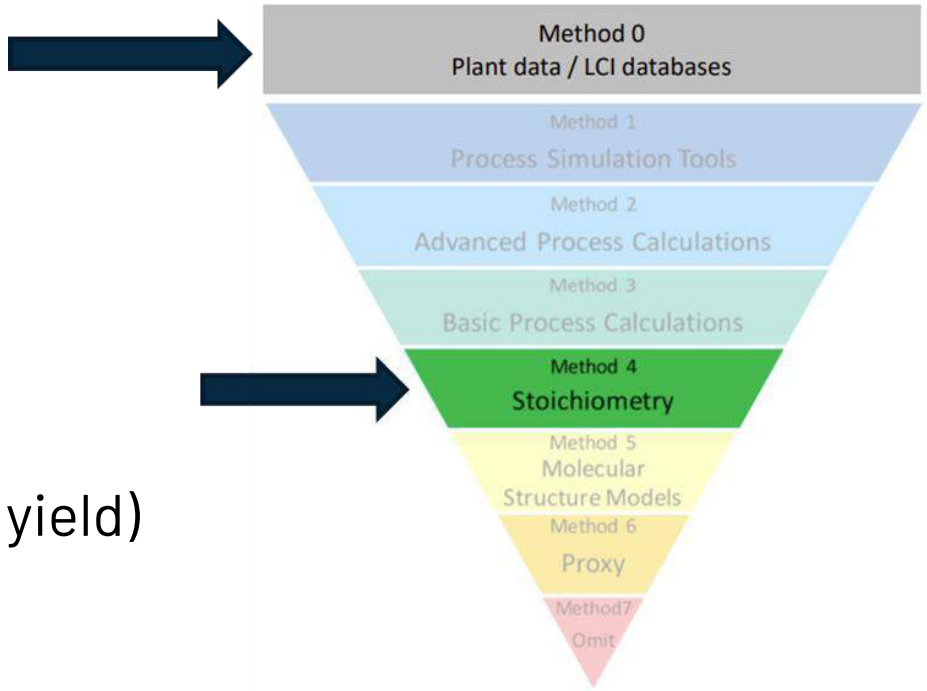
## How to fill data gaps (production)

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




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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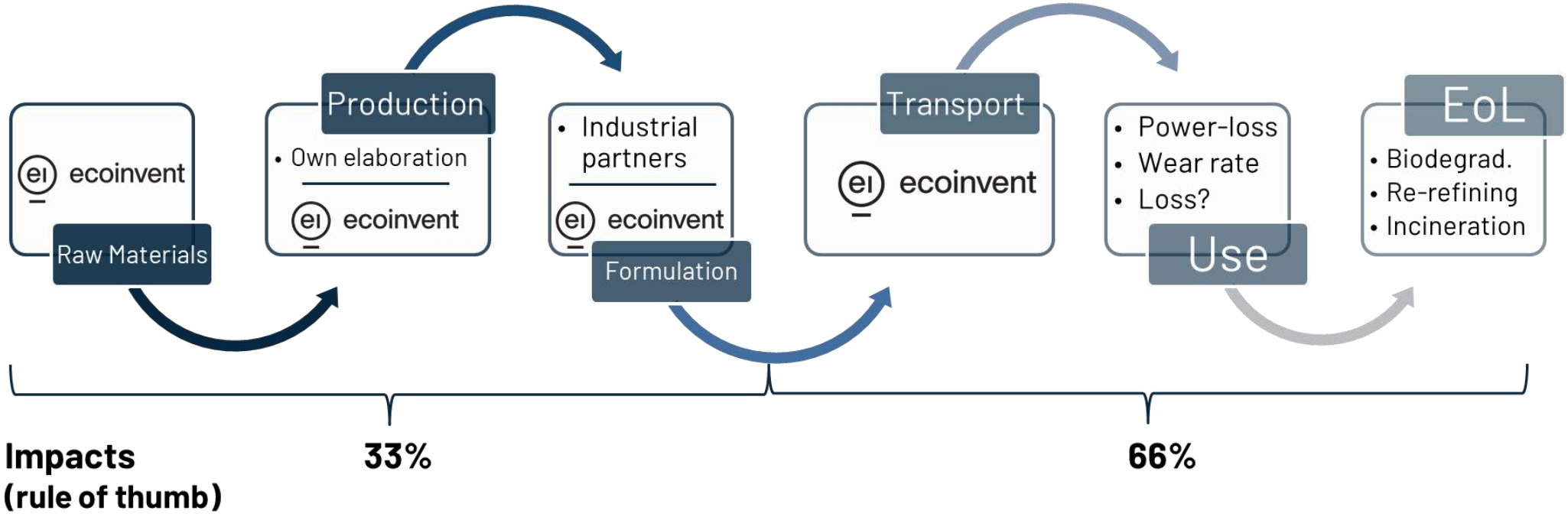
# Life Cycle Assessment (LCA) of lubricant components

## Life Cycle Stages (short)

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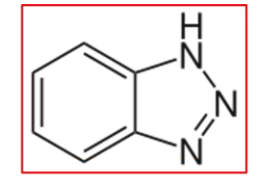
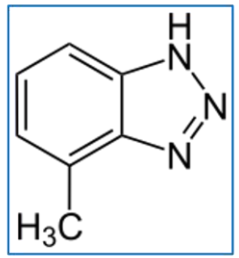
# Life Cycle Assessment (LCA) of lubricant components

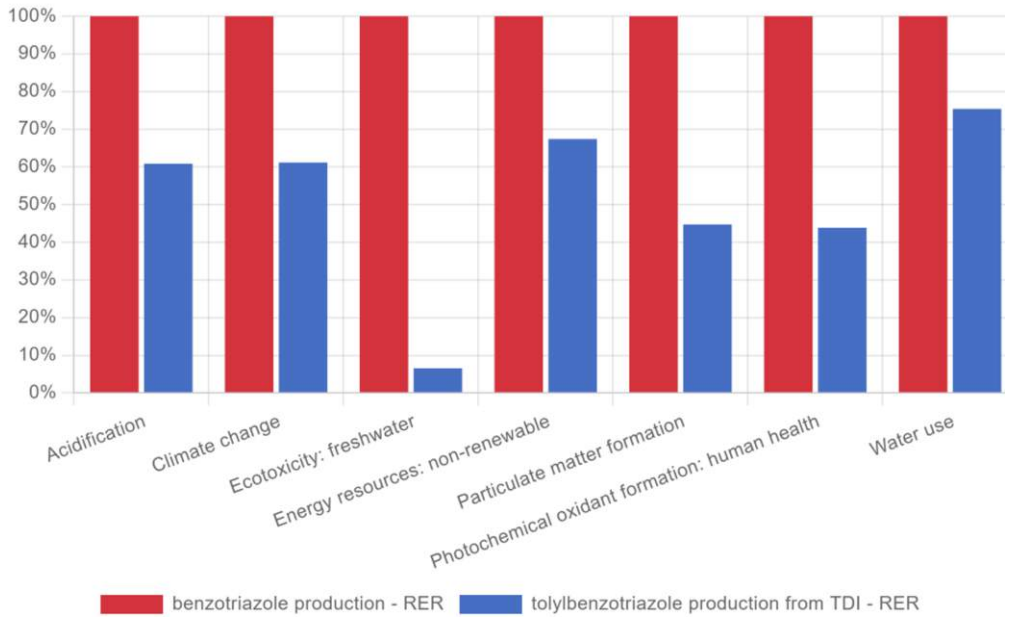
## SSbD case (Cradle-To-Gate)

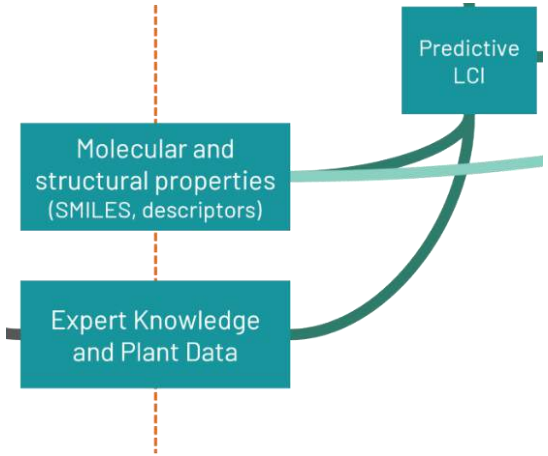


SSbD base case



SSbD alternative




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

Semi-automated process with expertise needed

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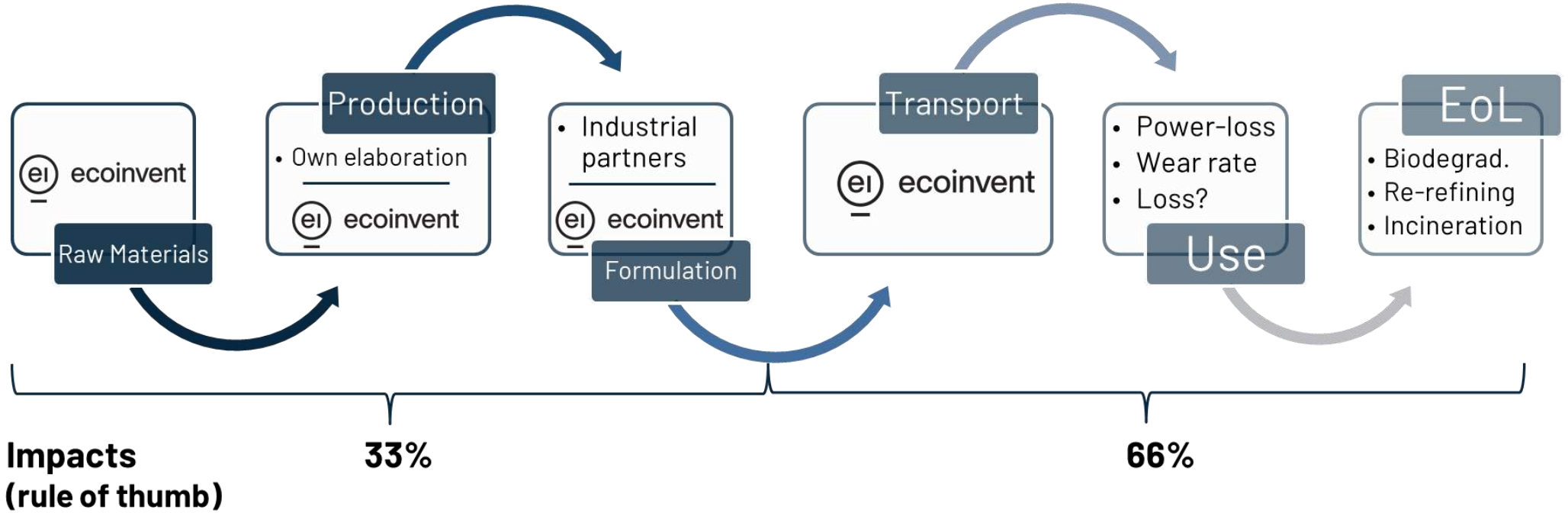
# Life Cycle Assessment (LCA) of lubricant components

## Life Cycle Stages (short)

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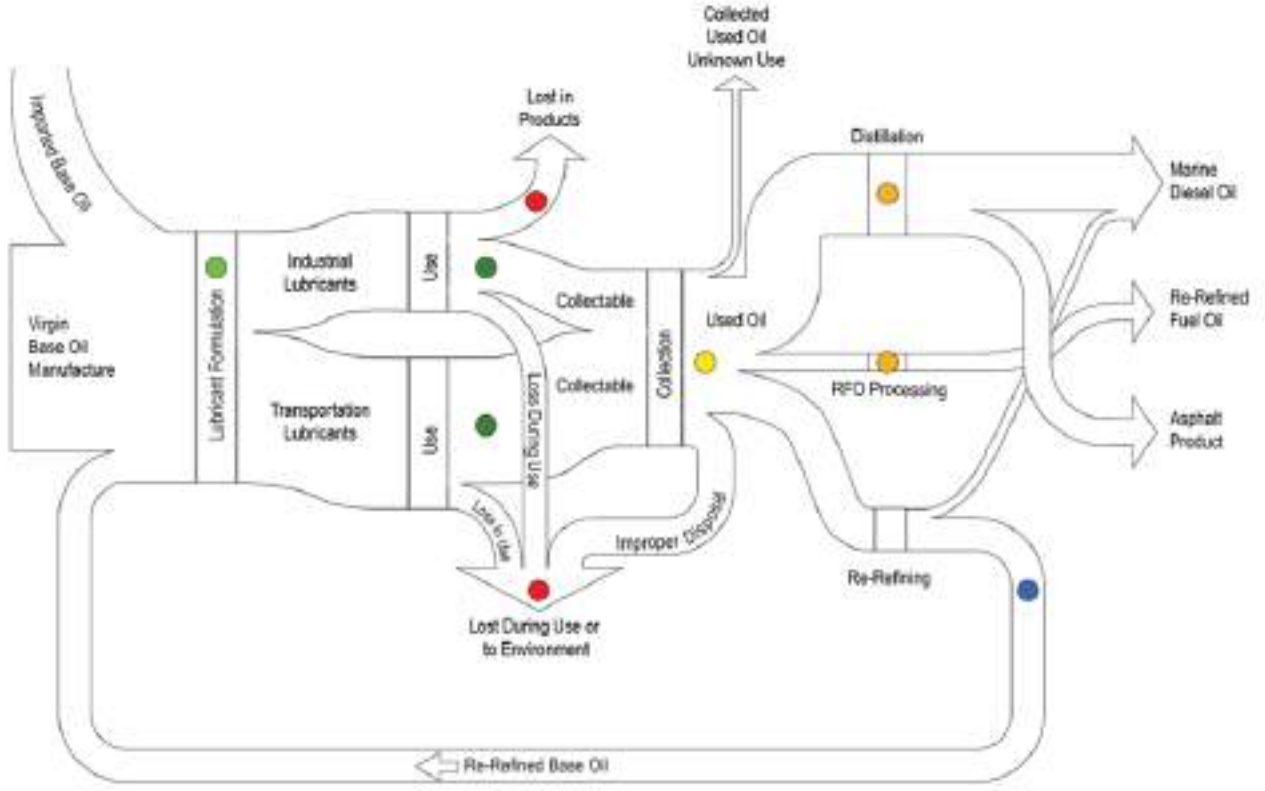
## End-of-Life for lubricants




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

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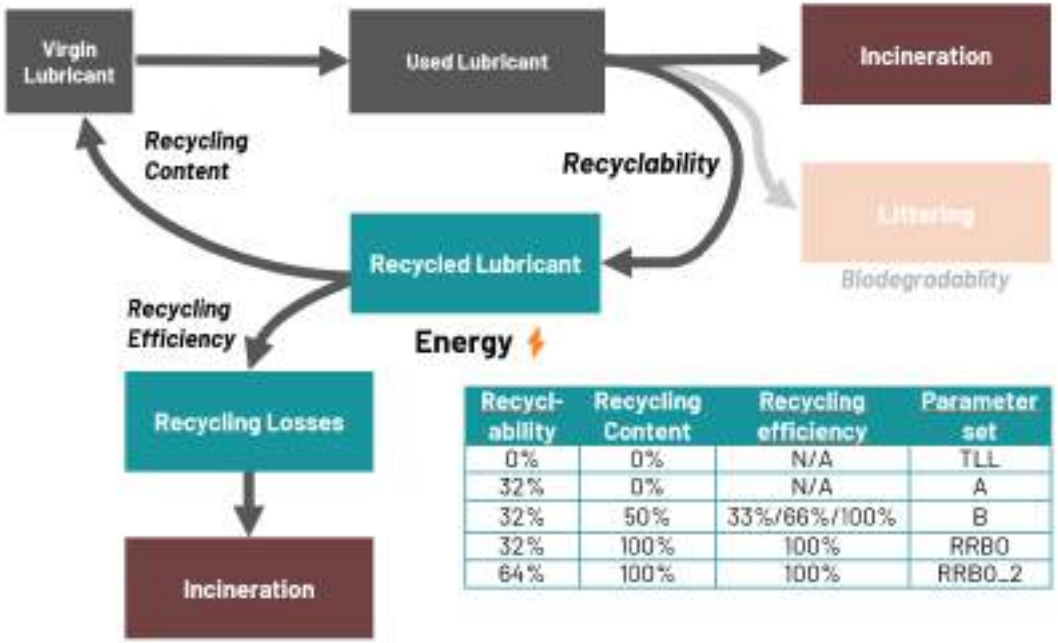
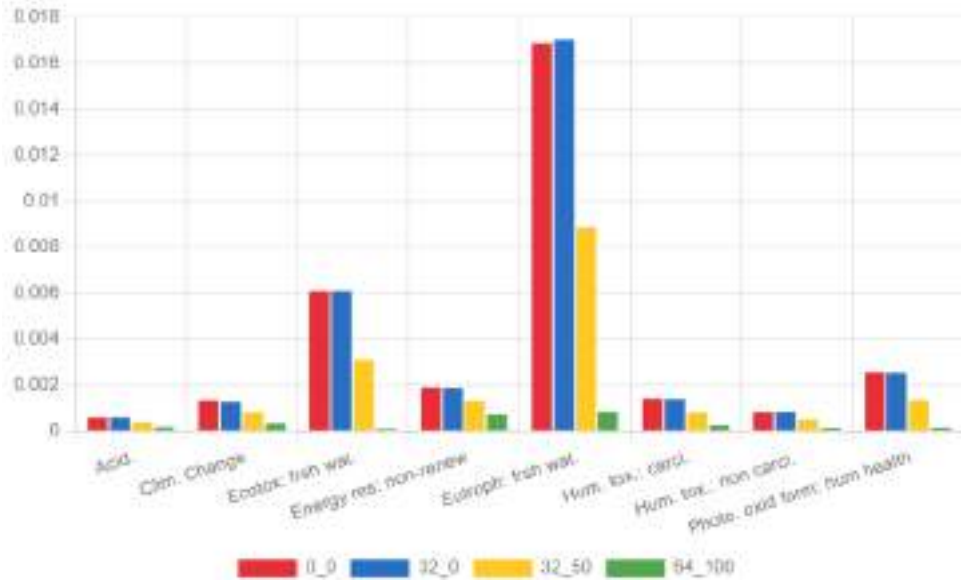
# Life Cycle Assessment (LCA) of lubricant components

## End-of-Life for lubricants




| Recycl-ability | Recycling Content | Recycling efficiency | Parameter set |
|---|---|---|---|
| 0% | 0% | N/A | TLL |
| 32% | 0% | N/A | A |
| 32% | 50% | 33%/66%/100% | B |
| 32% | 100% | 100% | RRB0 |
| 64% | 100% | 100% | RRB0_2 |




*Normalization bar chart for soybean-based lubricant with recycling as end-of-life scenario referenced to 1 kg, ecoinvent 3.10 cut-off, EF 3.1 method*

To predict EoL, 'parameter sets' can be used

→ Scenarios and legislation can guide us

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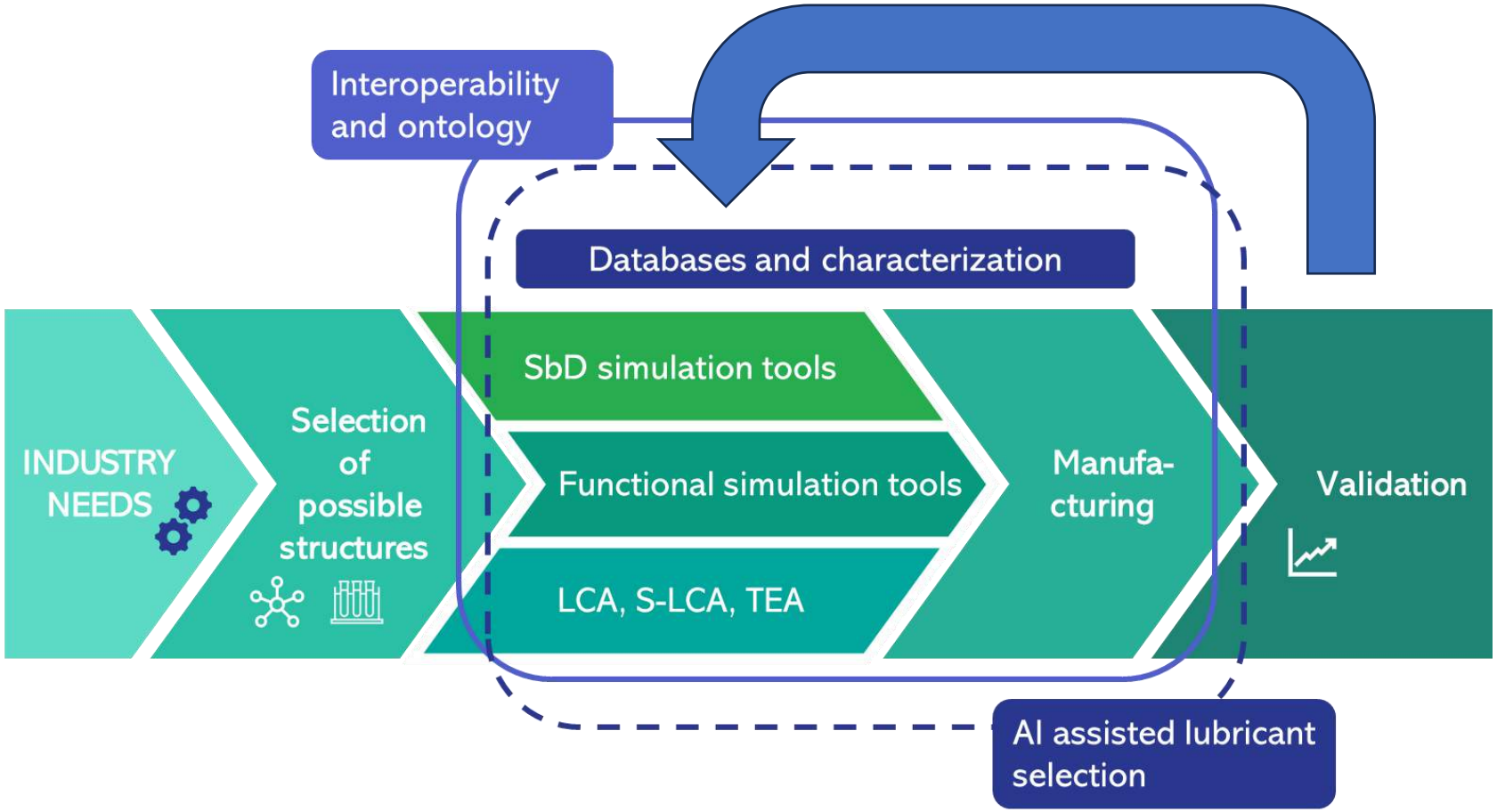
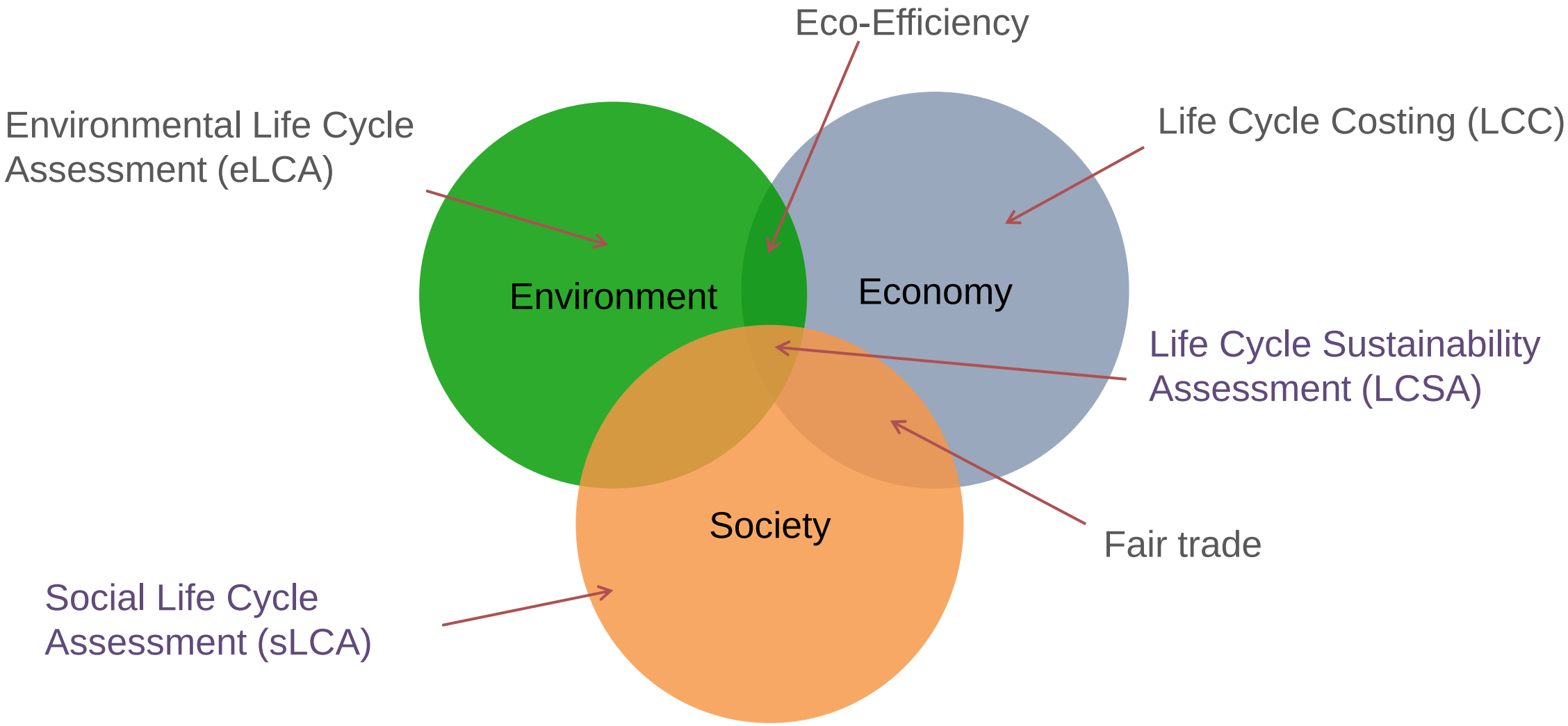
# SiToLub - WORKFLOW



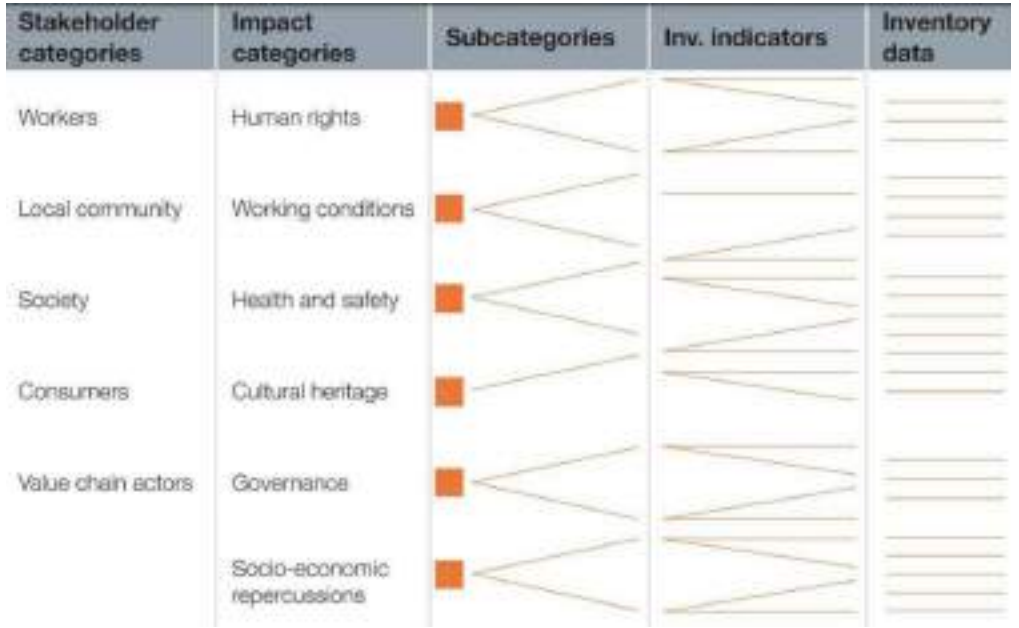

**Validation with experimental indication will improve the simulation!**

# More than environmental LCA → life cycle sustainability assessment



## Social LCA

- Technique to assesses social/socio-economic aspects and impacts
- aspects assessed in S-LCA (in)directly affect stakeholders positively or negatively during life cycle of product
- sLCA is no basis for decision if product should be produced or not, but
  - to detect social hotspots
  - instigate dialogue on social aspects of production and consumption
  - To improve performance of organizations and ultimately the well-being of stakeholders



## Social LCA and SSbD

- Social data is often qualitative → hard to access, measure and organize
- also assessment of data and impacts is subjective → different approaches, individual evaluation and interpretation → generic database approach (ILO)
- Social information changes fast → regular updates are needed
- GreenDelta developed a social database (2017):

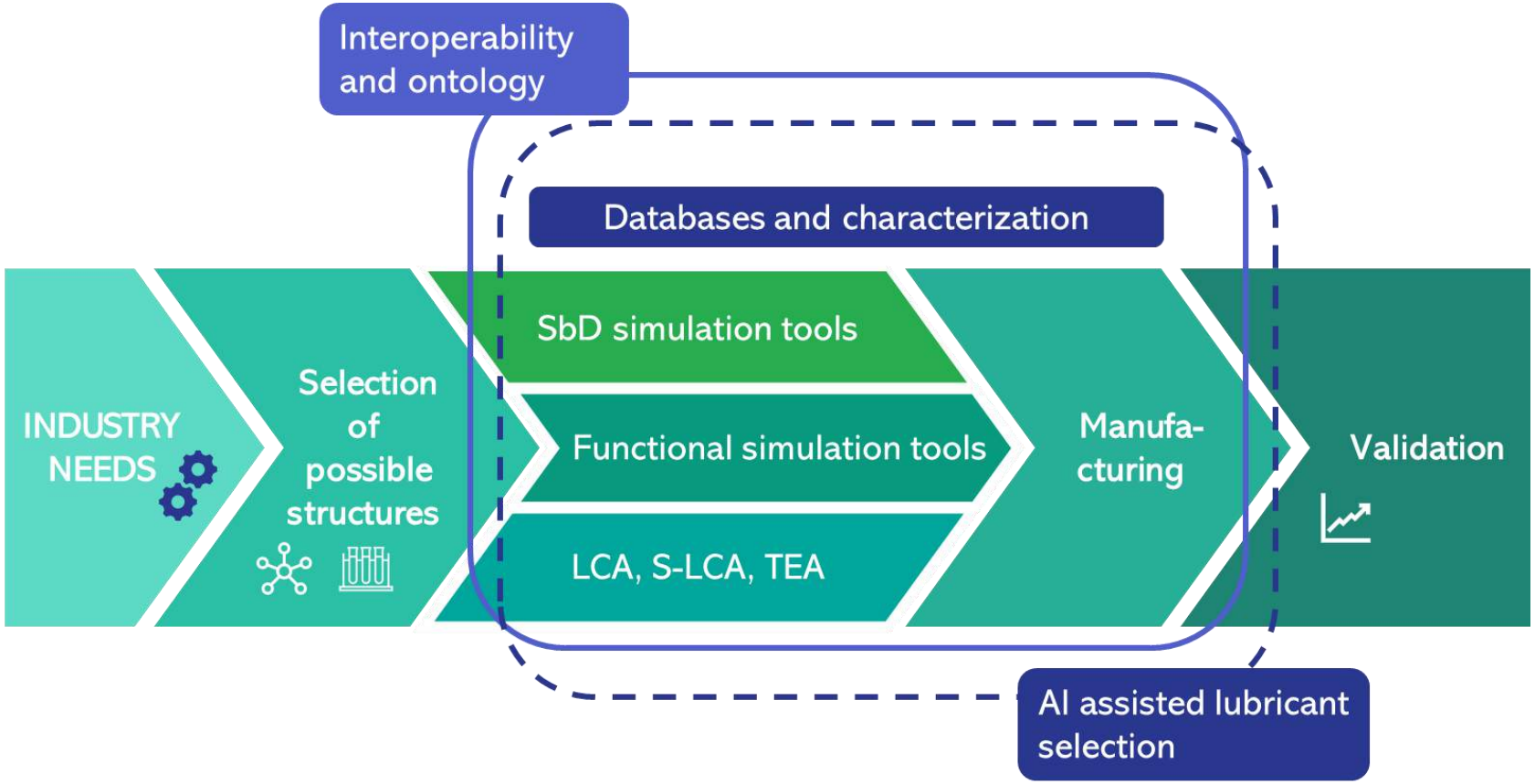
PSILCA

- allows calculation and assessment of the social impacts of products along the products' entire life cycles and to detect social hotspots
- Has been used by JRC for the SSbD case studies for 'stage 5'



More information at www.PSILCA.net

# SiToLub - WORKFLOW




Market

# Recap – SSbD lubricants

- Lubricants aid sustainability by lower friction and heat losses in energy
- Industry is seeking for new products that are safe by design
  - No GHS, low price, high performance, no SHVCs, no allergens, low PCF..
- SSbD approach gives rise to novel R&D principles during the design
  - Life cycle thinking
- In SiToLub we try to simulate and validate novel SSbD-lubricants
  - Combination of QSAR and performance simulation feeds eLCA
  - Predictive eLCA will simulate environmental impacts (full life cycle)
  - Social LCA can be integrated in SSbD criteria (PSILCA)

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SiToLub

# CONTACT

Dr. Jonas Hoffmann
GreenDelta GmbH
**hoffmann@greendelta.com**

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