GreenDelta
sustainability consulting + software

openLCA

From Carbon to Multi-Criteria Decisions: Making Sustainability Assessment Actionable for Circular Chemistry

Picture: Julia Cilleruelo Palomero

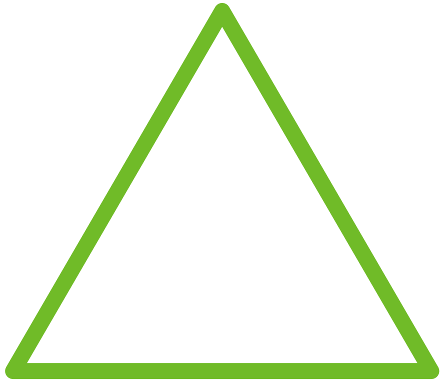
Dr. Jonas Hoffmann, Julia Cilleruelo Palomero, GreenDelta GmbH, Berlin
on 06th July, 2026, CTC Focus Day

GreenDelta, What we do

- 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, Life Cycle Costing, Circular Economy



openLCA nexus

Database development and distribution

openLCA

Software development, especially open source

About openLCA

openLCA

- Free and open-source project
- Developed by GreenDelta since 2007
- Constant development, continues updates
- Database flexibility and multifunctional
  - LCA, LCC, Social LCA and LCSA
  - Carbon & Water footprint
  - Product Environmental Footprint (PEF)
  - Environmental Product Declarations (EPDs)

2.6.2

- Better system dynamics tooling (needs to be enabled under experimental features File > Preferences > Experimental features)
  - Full graphical editor for variables and product system bindings
  - Usage of XMILE as data exchange format
- Fix: Regionalized LCIA missed some flows with some location combinations
- Fix: Monte Carlo Simulation did not include linked results. Further the respective error dialog got improved

2.6.1:

- Improved user interface, including a resized search box for certain display resolutions and a refined dark mode theme
- Major memory reduction for regionalized LCIA, resulting in smoother performance and making calculations more accessible for users with limited system resources
- Faster calculations overall, including direct impact calculations
- Bug fixes from v2.6.0 for a smoother user experience
- Easier deletion of process chains in the graphical editor (Model Graph)
- Better support for opening Python scripts on macOS and Linux

2.6.0:

- System Dynamics (SD) simulation and modeling (experimental feature)
- Hestia import functionality with flow mapping selection and data preview
- Improved Jython/Python integration: CodeMirror 6 editor with code completion and run keymap
- Library signing (experimental)
- GLAD mapping file import support
- Allow results as default providers in processes with drag and drop support
- Allow adding multiple impact categories and flows to results at once
- Better provider names in Sankey diagram
- Improved process names in model graph
- Social aspects: allow deletion of a set of indicators under social aspects tab
- Fix: direct impacts of processes
- Fix: deletion of database repository
- Fix: library signing UI issues

https://www.openlca.org/download/

GreenDelta, Research Activity

https://www.greendelta.com/projects/

PRIMUS

Sustainability of Plastic Recylates

TriFluorium
safe fluorine circularity

Sustainability of Fluoropolymer Tribolysis

MOST-H_2

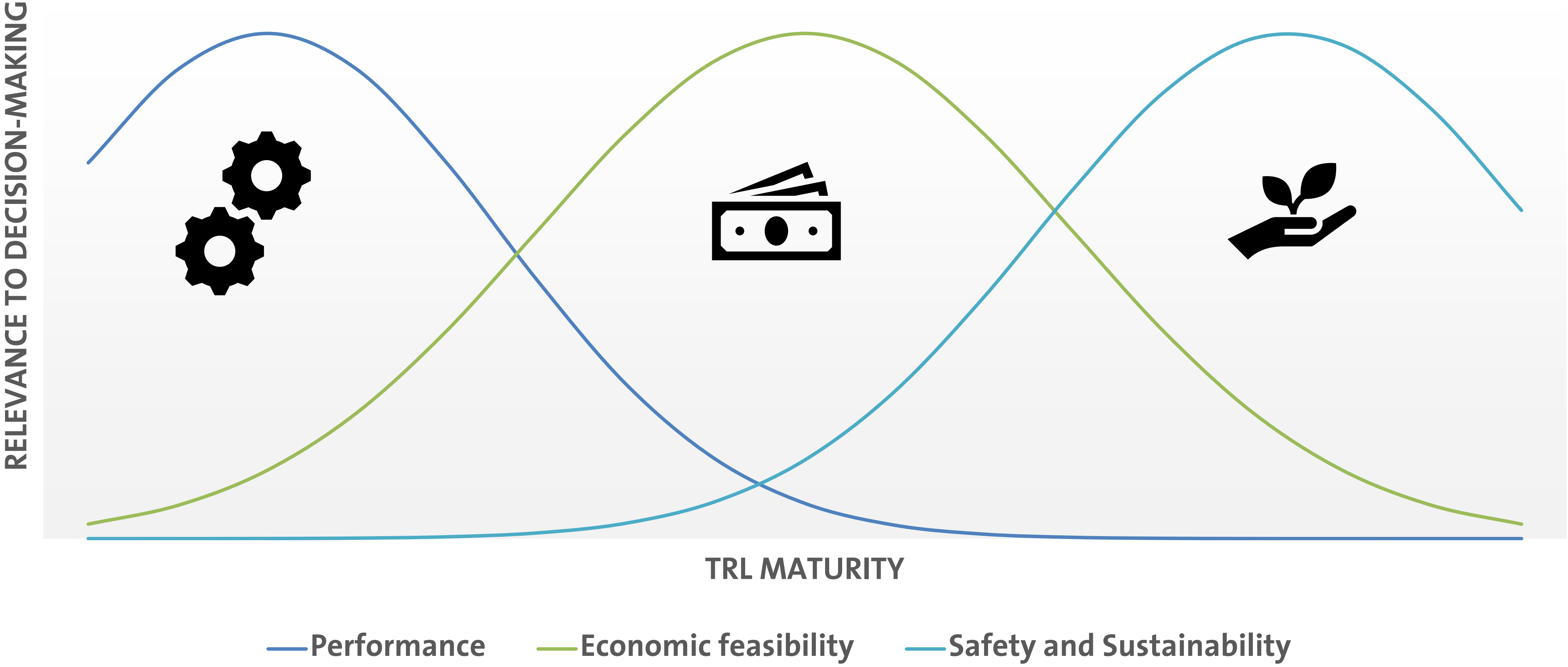
Sustainability of MOFs for H_2 storage

SITOLUB

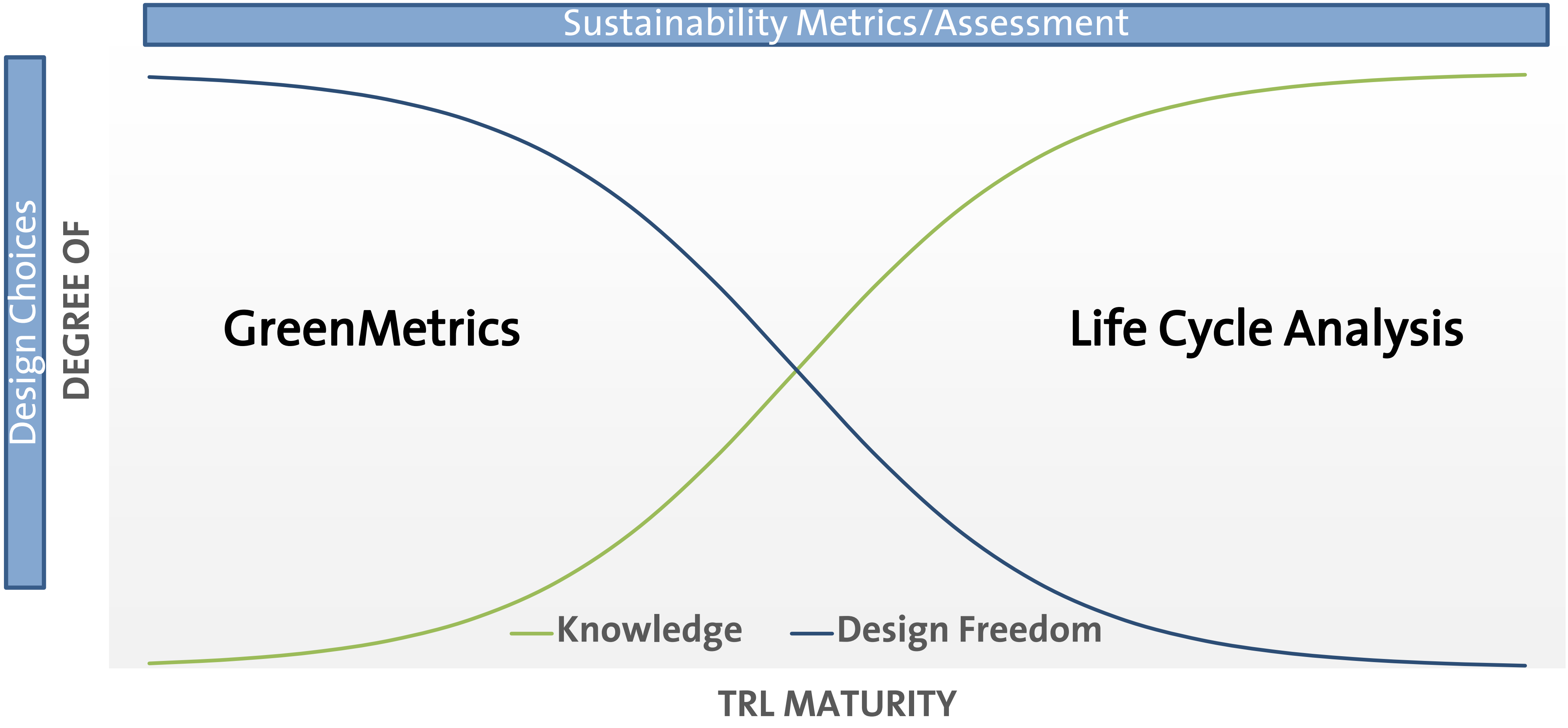
Sustainability Simulation for novel SSbD lubricants

How to assess the sustainability at low TRL?

Innovation of Chemicals



Sustainable Chemistry, Design Criteria



See Blömer et al., Chem. Ing. Tek. 2024, 96, 561-574 and Wu et al. Chem. Circ. 2026, 100080.

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Sustainable Chemistry, Design Criteria

Green Chemistry:

1. Prevent waste
2. Maximize atom economy
3. Design less hazardous chemical syntheses
4. Design safer chemicals and products
5. Use safer solvents and auxiliaries
6. Increase energy efficiency
7. Use renewable feedstocks
8. Reduce derivatives
9. Use catalysts
10. Design for degradation
11. Real-time analysis for pollution prevention
12. Inherently safer chemistry for accident prevention

Circular Chemistry:

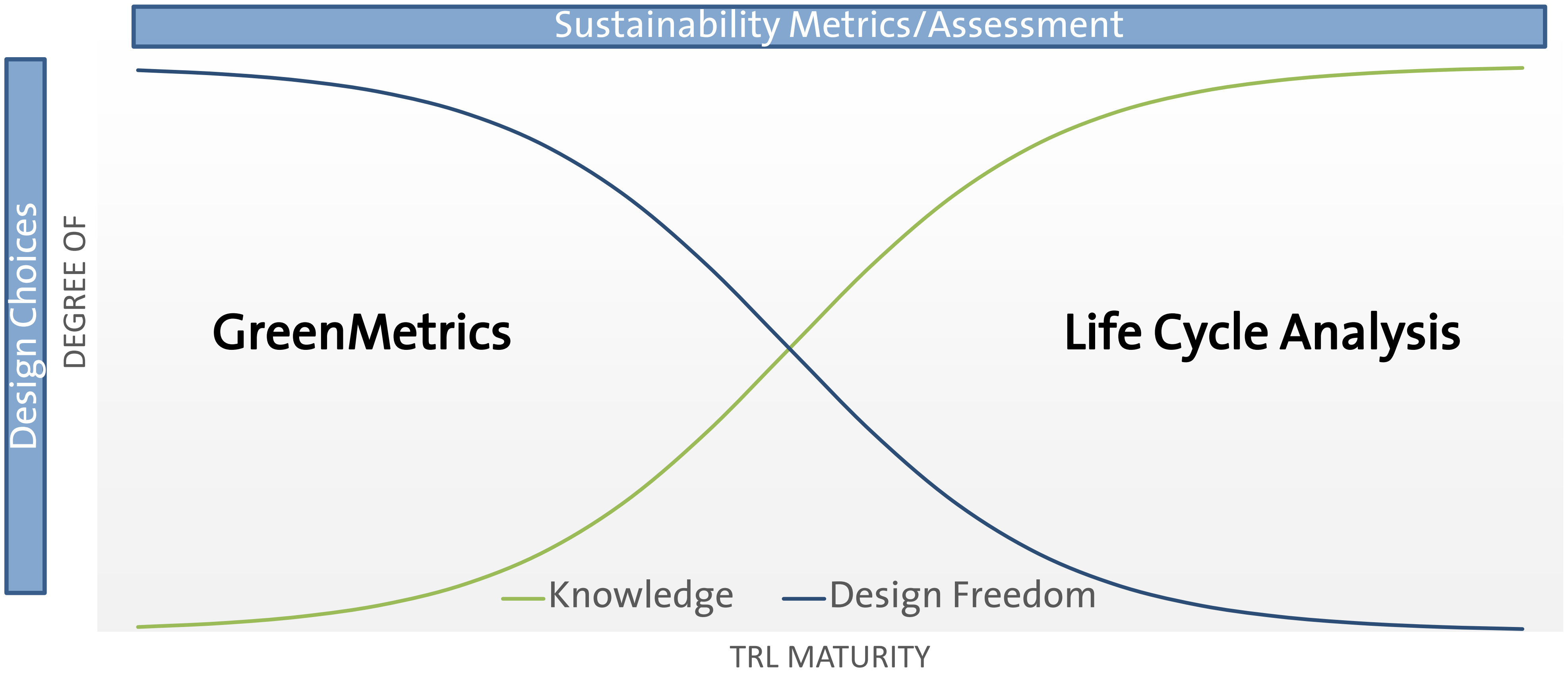
1. Collect and use waste
2. Maximize atom circulation
3. Optimize resource efficiency
4. Strive for energy persistence
5. Enhance process efficiency
6. Avoid out-of-plant toxicity
7. Design for optimal end-of-life
8. **Assess sustainability across the life cycle**
9. Apply the ladder of circularity
10. Sell service, not product
11. Reject lock-in
12. Unite industry with coherent policy

SSbD design criteria:

1. Material efficiency
2. Minimise the use of hazardous chemicals/materials
3. Design for energy efficiency
4. Use renewable sources
5. Prevent and avoid hazardous emissions
6. Reduce exposure to hazardous substances
7. Design for end-of-life
8. Consider the whole life cycle
9. Ensure responsible sourcing and minimise social risks

See Anastas and Warner, Green Chemistry: Theory and Practice; Keijer et al., Nature Chemistry 2019, 11, 190–195; and JRC, Safe and Sustainable by Design Chemicals and Materials.

GreenDelta, Design Criteria



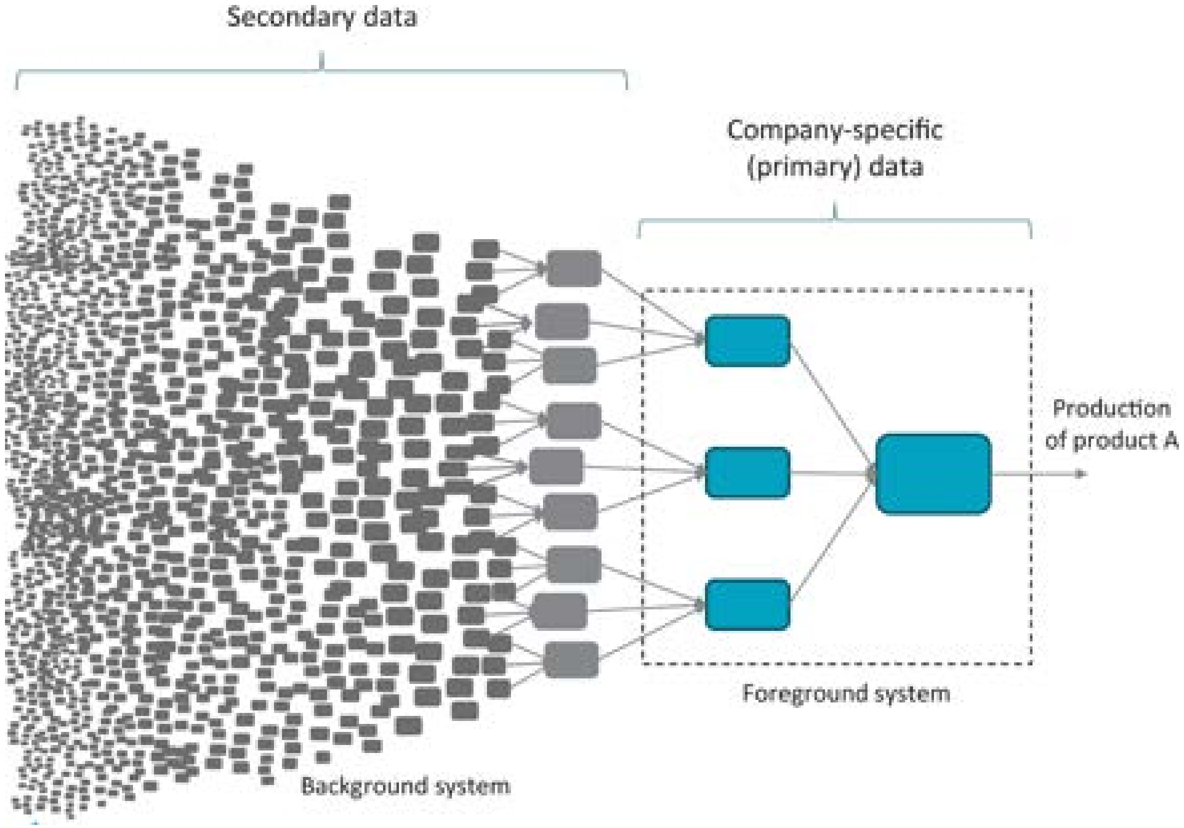
See Blömer et al., Chem. Ing. Tek. 2024, 96, 561-574 and Wu et al. Chem. Circ. 2026, 100080.

Foreground, Background

Quantifiable indicators (SSbD framework):

Indicator	Best case	Worst case
Net mass of materials consumed (kg/kg)	1	0.4
Reaction Yield (%)	100	40
Atom Economy (MProduct/MWtotal reaction)	100	
Material Intensity index (kg materials / kg product)	1	
Recycling efficiency/recovery rate (%)	100	
Critical Raw Material presence (yes/no + amount)	0	1
Biodegradability of manufactured chemical/Material	1	0
Classification of raw chemicals/materials as SVHC (yes/no + amount)	0	1
Yield of extraction (mass of recovered solvent / used solvent)	1	0
Renewable or fossil feedstock (yes/no + amount)	1	0
Recycled content (%)	100	0
Share of Renewable Energy (%)	100	0
Amount of hazardous waste (kg/kg)	0	1
Biodegradability of manufactured chemical	1	0

This is only the foreground!



The whole supply chain counts!

Chart from Rognan et al. 2025 J. Ind. Ecol. 29, 1397–1413.

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Foreground, Background

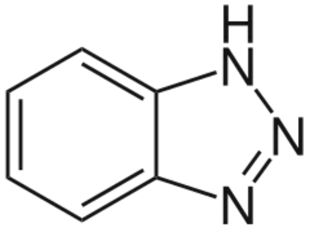
- Using modification of background databases, we can assess more dimensions:

Circularity across Life Cycle:
- Material Circularity Index
- Circularity Index

Criticality and SVHC usage across Life Cycyle:
- Inventory along the supply chain
- Weighting (SH2E method) for CRMs

Plastic Littering:
- Based on a probalistic model

Foreground, Background: Criticality



Benzotriazole

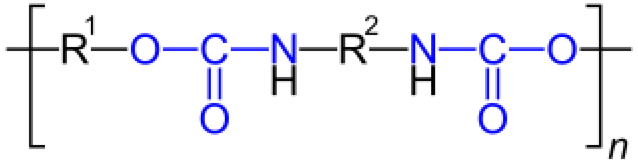
Indicator	Best case	Worst case
Critical Raw Material presence (yes/no + amount)	0	1

- Criticality investigates the usages of CRM and SRM (by EU definition)
- **SRMs**: Arsenic, Coking Coal, Feldspar, Helium, Lithium, Manganese, Copper, Nickel
- We added shadow flows in the DB and added SH2E CFs to assess the Criticality

Name	Inventory result	Characterization factor	Impact assessment result
SSbD CRM with SH2E CFs with Jonas Shad			4.84386E-11 dimensionless
Coking Coal CRM	0.28106 kg	6.87000E-11 dimensionless/kg	1.93086E-11 dimensionless
Magnesium CRM	4.71253E-5 kg	2.62000E-7 dimensionless/kg	1.23468E-11 dimensionless
Boron CRM	3.70782E-7 kg	1.92000E-5 dimensionless/kg	7.11902E-12 dimensionless
Manganese CRM	9.46466E-5 kg	3.51000E-8 dimensionless/kg	3.32209E-12 dimensionless
Nickel CRM	0.00034 kg	5.26000E-9 dimensionless/kg	1.80458E-12 dimensionless

- CFs (here criticality indicator) considers Supply Risk (SR), material consumption (C) in the EU, import reliance (IR), and the recycling input rate (EoL_{RIR})

Foreground, Background: SVHC



TDI-based polyurethane

Indicator	Best case	Worst case
Classification of raw chemicals/materials as SVHC (yes/no + amount)	0	1

- SVHCs are identified under **Article 57 of the REACH Regulation** and the list of SVHCs is maintained by the ECHA and holds currently 250 substances
- Tracking **complements** conventional **environmental impact indicators**

Name	Inventory r...	Impact assessment result
SSbD SVHC		0.74156 kg SVHC
SVHC - propylene oxide, liquid	0.52186 kg	0.52186 kg SVHC
SVHC - 2,4-dinitrotoluene	0.15911 kg	0.15911 kg SVHC
SVHC - triphenyl phosphate	0.04105 kg	0.04105 kg SVHC
SVHC - melamine	0.01796 kg	0.01796 kg SVHC

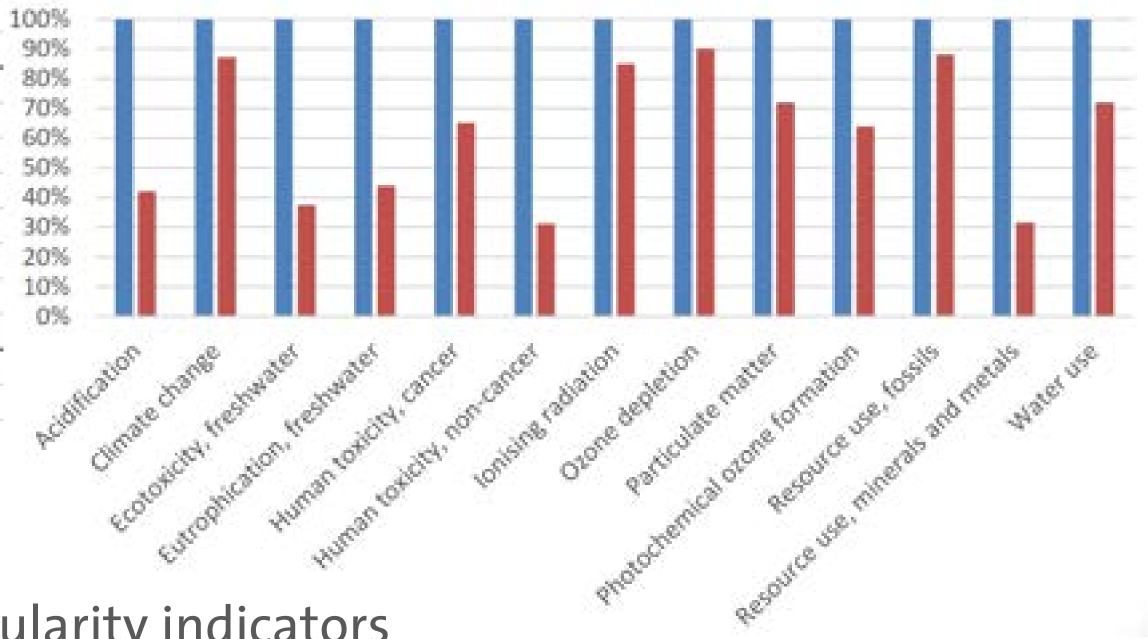
- Implementation of shadow flows allows analysis over the life cycle

Foreground, **Background: Circularity**

Indicator	Best case	Worst case
Recycled content (%)	100	0
Recycling efficiency/recovery rate (%)	100	

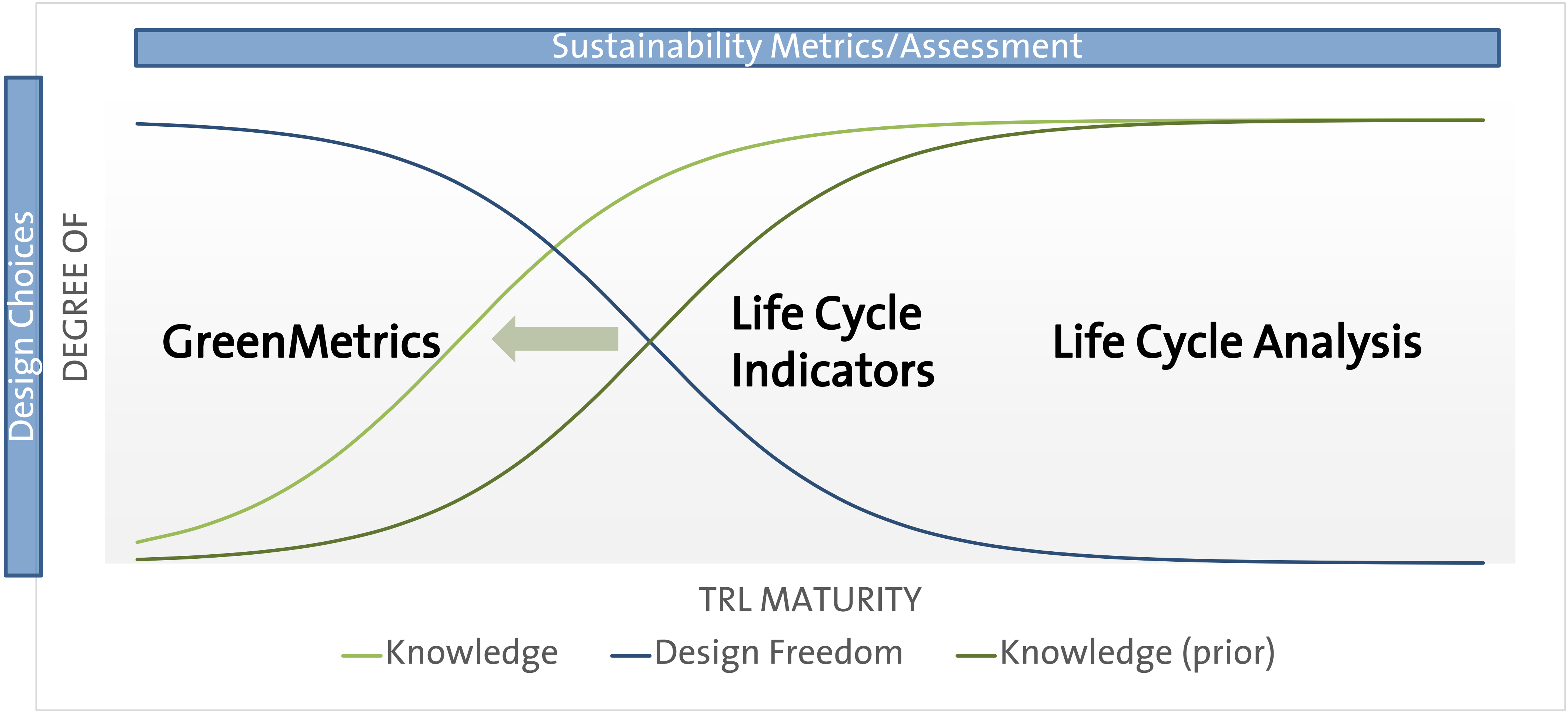
- Circularity is assessed across the life cycle using MCI and CI indicators
- Considering a battery production, Li-ion, rechargeable with 50% recycled copper:

	Base case	Improved case	
Name	Impact assessment result		Unit
energy required for primary production	17095.4	14242.8	MJ
energy required for recycled production	277.5	115.3	MJ
recovered EoL material	356.3	327.1	kg
recycled material	-160.7	-168.9	kg
total waste produced (W)	41604.5	15815.8	kg
virgin material (V)	19676.4	7292.6	kg
waste from recycling processes (Wc)	36.5	27.8	kg
waste from the production of secondary feedstock, (Wf)	0.3	0.3	kg
MCI (from LCA)	0.11652	0.13807	
CI (from LCA)	0.01764	0.04355	



- Here, environmental impacts follow the circularity indicators

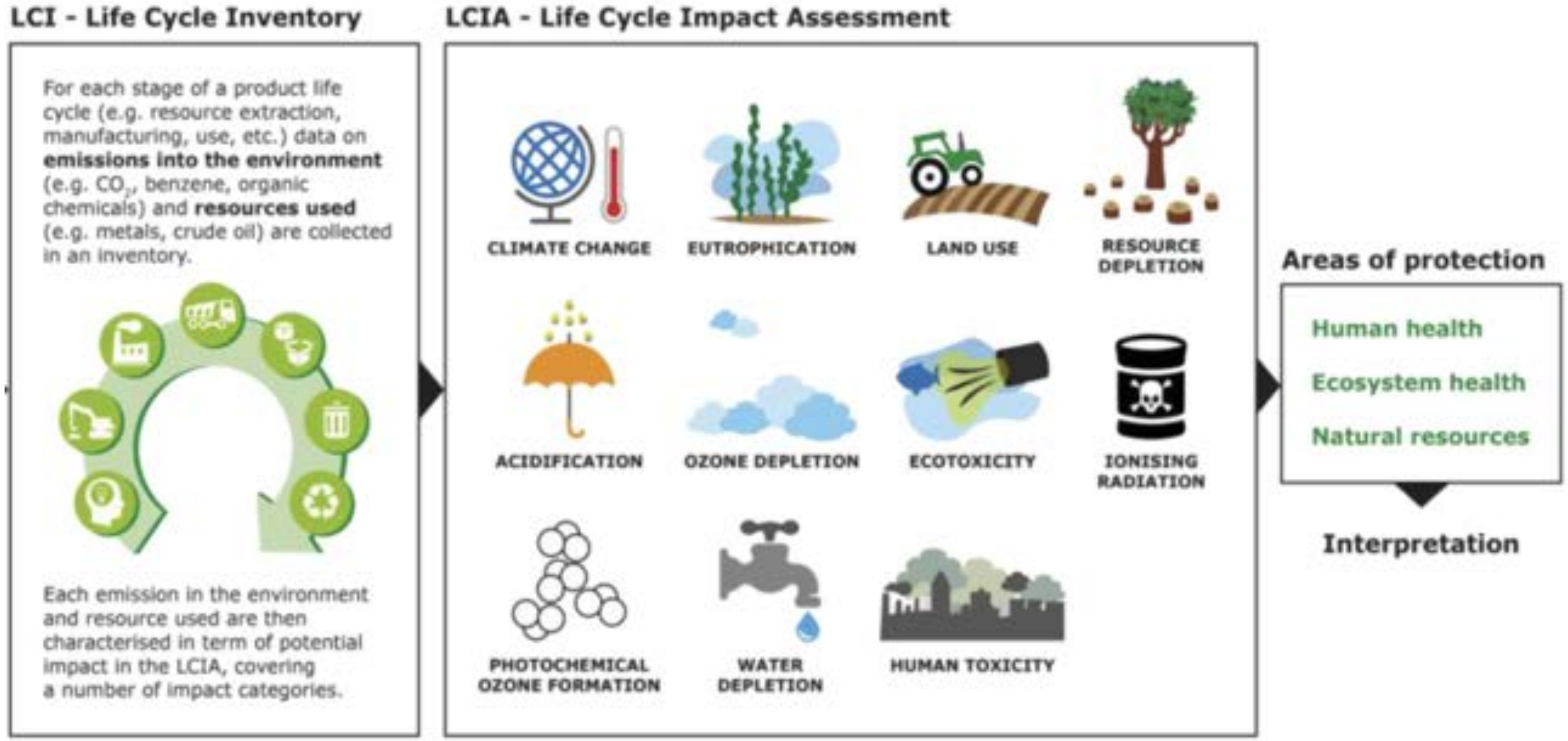
Design Criteria: Shifting



How to conduct an LCA for chemicals on low TRL?

What is even: Life Cycle Analysis

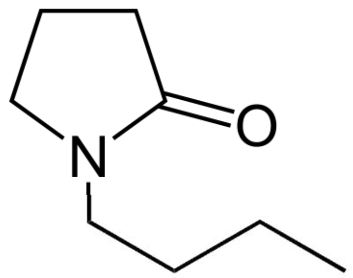
Definition (DIN 14044): *'Life Cycle Assessment (LCA) is a compilation and evaluation of inputs, outputs and the potential environmental impacts of a product system through its life cycle.'*



LCA is attempting to prevent *trade-offs but often based on secondary data*

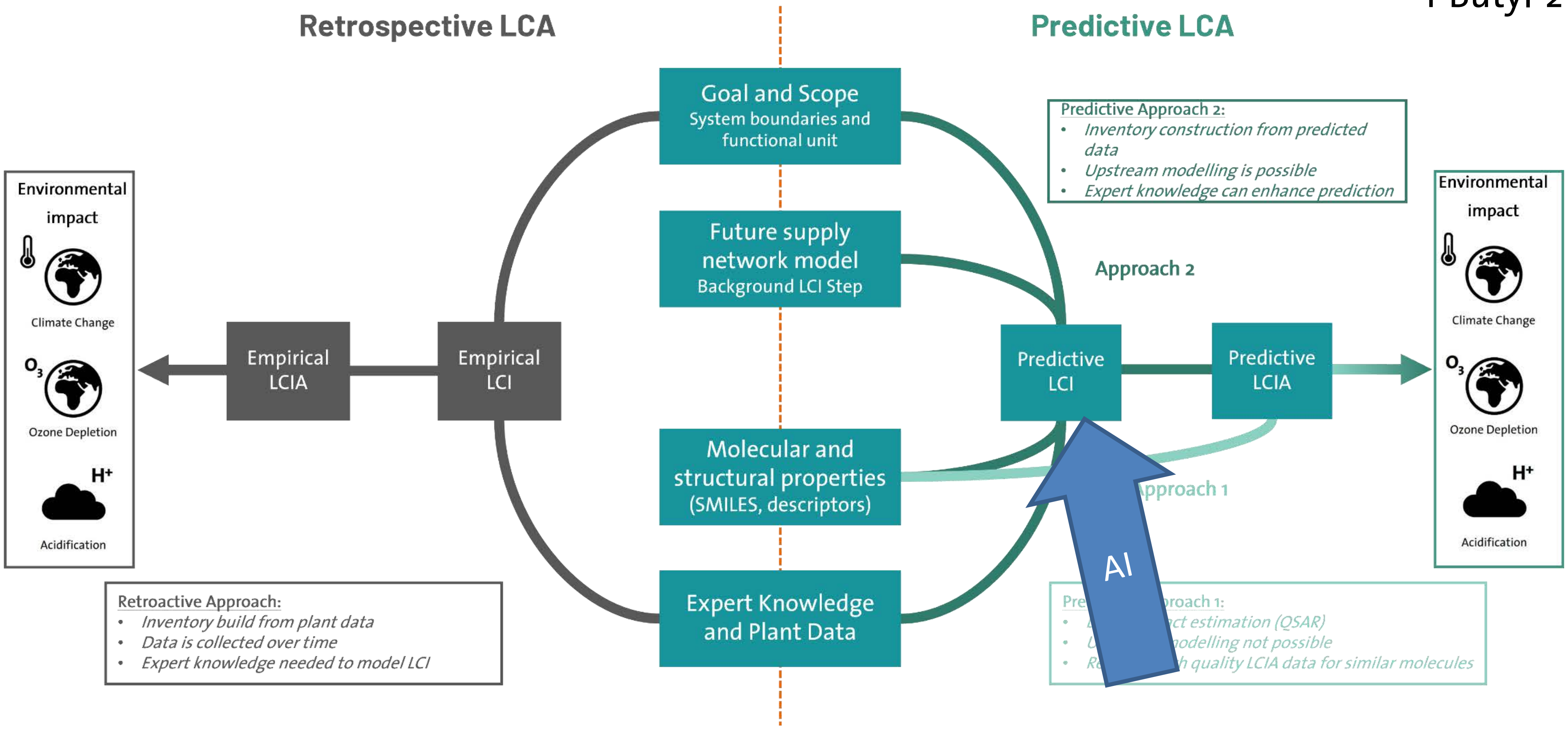
Sala S., Cerutti A.K., Pant R., Development of a weighting approach for the Environmental Footprint, Publications Office of the European Union, Luxembourg, 2018, ISBN 978-92-79-68042-7, EUR 28562, doi:10.2760/945290

Foreground, Background: Data Gaps

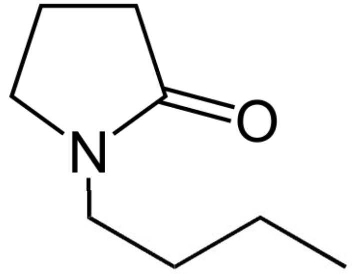


1-Butyl-2-pyrrolidone

- How to obtain data for speciality chemicals?

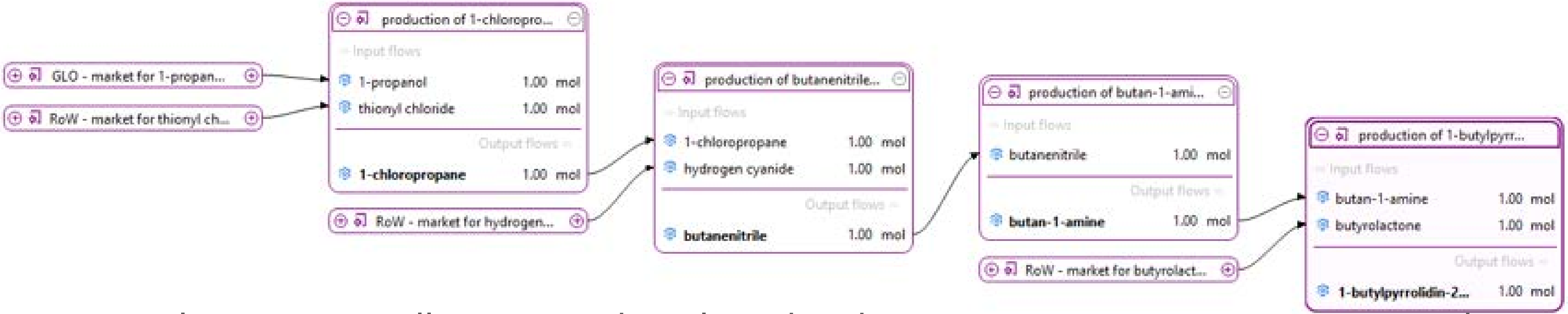


Foreground, Background: Data Gaps



1-Butyl-2-pyrrolidone

- Trend to implement AI as part of LLMs in LCA but it is limited with chemicals
- 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
- Covers only production with generic assumptions, **full life cycle is relevant**!

https://github.com/GreenDelta/retrolca

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Drawing the full sustainability picture

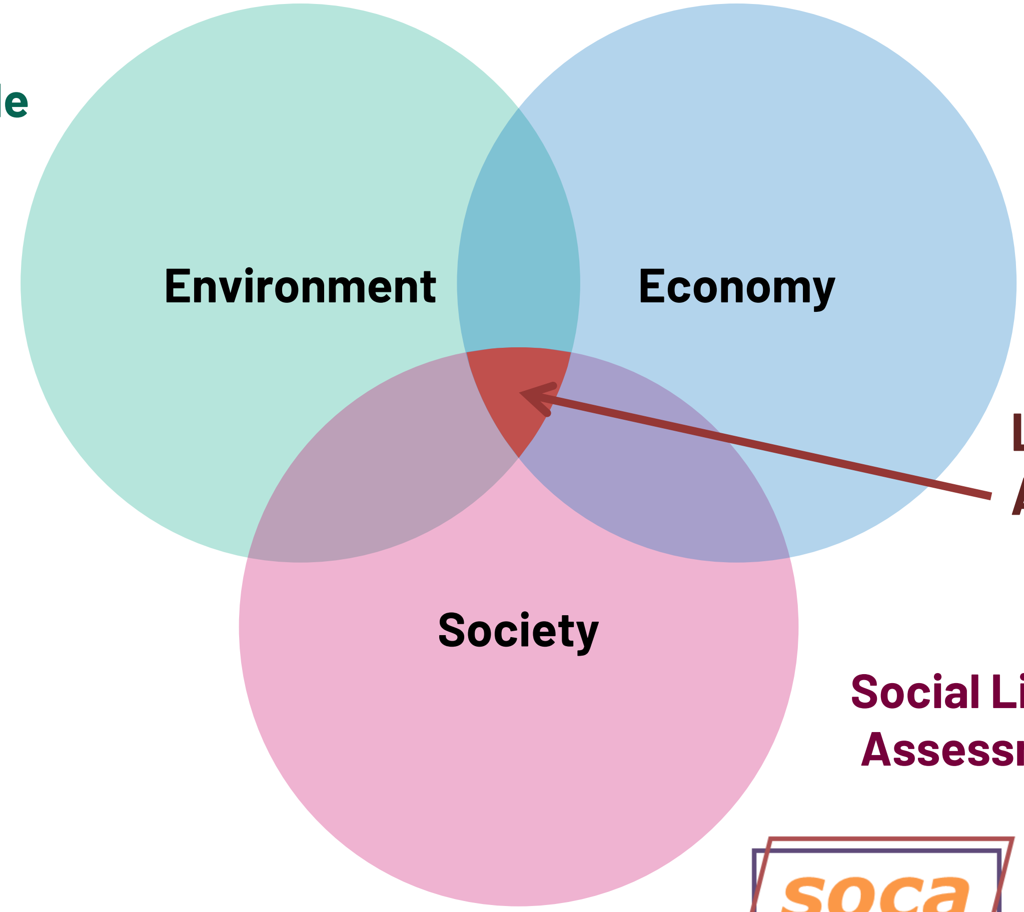
Environmental Life Cycle Assessment (eLCA)

ecoinvent

Bundesamt für Umwelt BAFU

carbonminds

Circularity package



Life Cycle Costing (LCC)

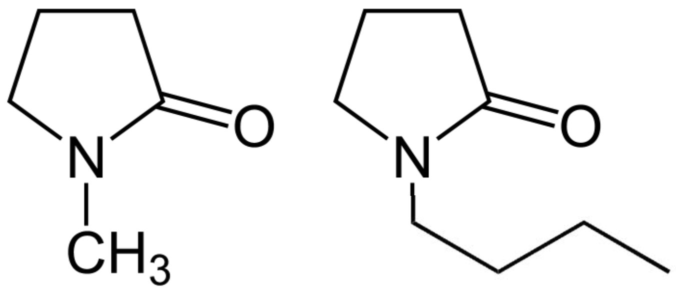
Life Cycle Sustainability Assessment (LCSA)

Social Life Cycle Assessment (sLCA)

soca

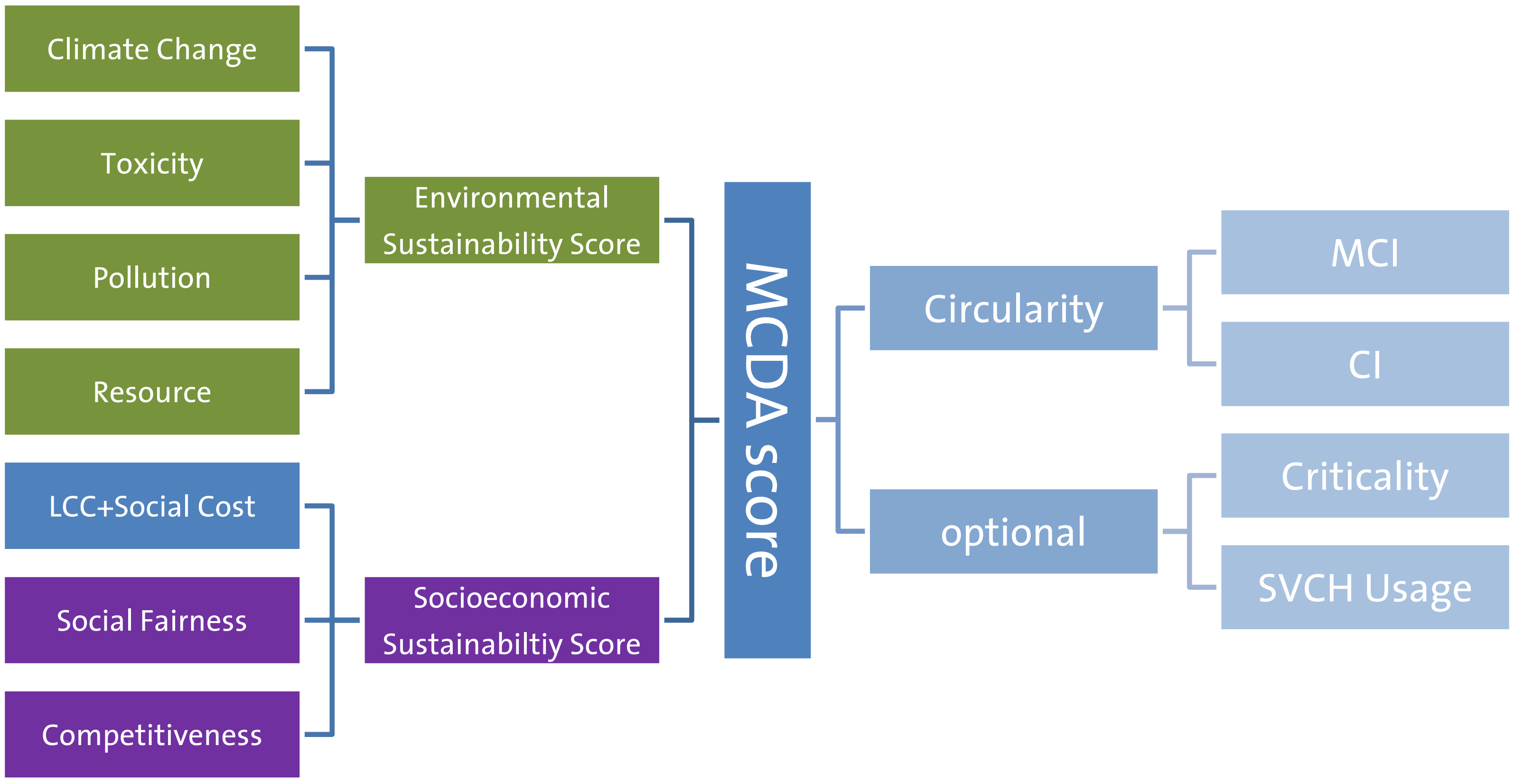
PSILca

Drawing the full sustainability picture



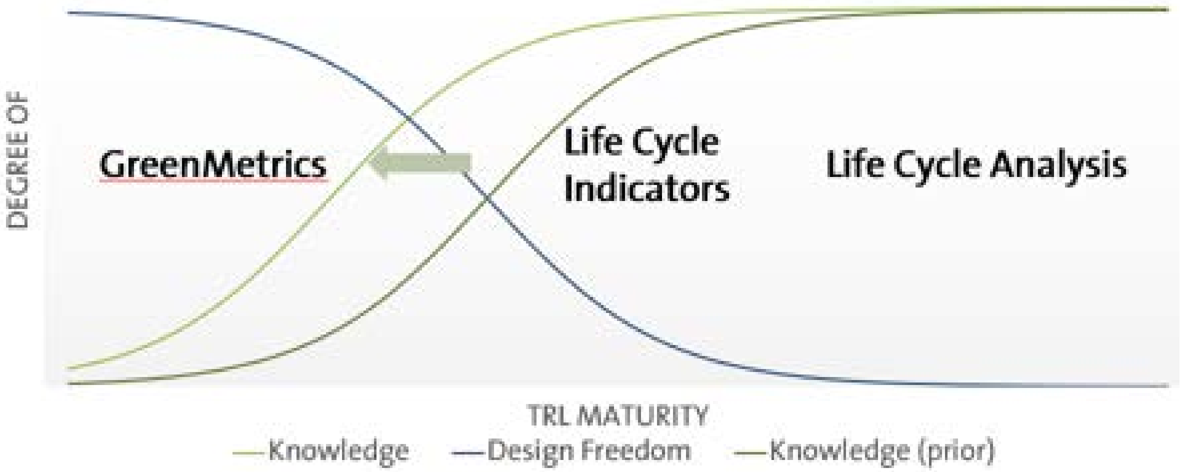
NMP

1-Butyl-2-pyrrolidone



- Integrating **indicator-based results** into decision-making at low TRLs can facilitate early-stage decision-making
- However, distinct **uncertainty analysis** and data quality must be considered

Key takeaways



- Design criteria/metrics in chemistry should cover the entire life cycle (**foreground and background** systems)
- With **data solutions**, we can support decision making at early stage
  - Transparent LCI databases serve as basis for **indicator-based** frameworks (circularity, criticality, SVHC) to make **early design choices actionable**
  - **openLCA with retrolca implementation** allows retrosynthetic LCIs and closes data gaps for chemicals **allowing decision making on R&D level**
- Full sustainability requires LCSA for the entire life cycle (cradle-to-grave)

We are open for collaboration on research and innovation projects in Circular Chemistry an Safe-and-Sustainable-by-Design

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openLCA

Thank you!

Picture: Julia Cilleruelo Palomero

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