Digital Sustainability Tools for Future Chemicals and Fuels

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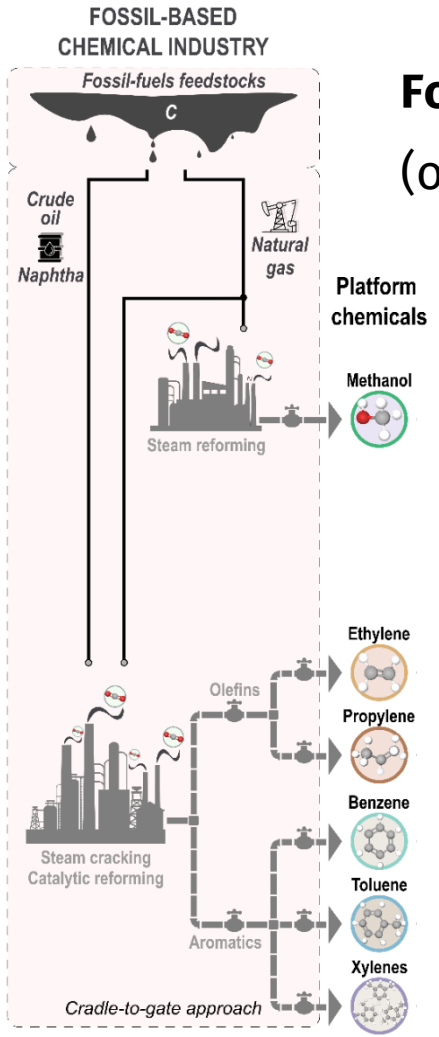
ecoinvent

ETH zürich

Current fossil-based chemical industry is unsustainable



Fossil carbon

(oil and natural gas)

C

CO_2

CO_2

CO_2 (CCU)

Biomass

Chemical products waste

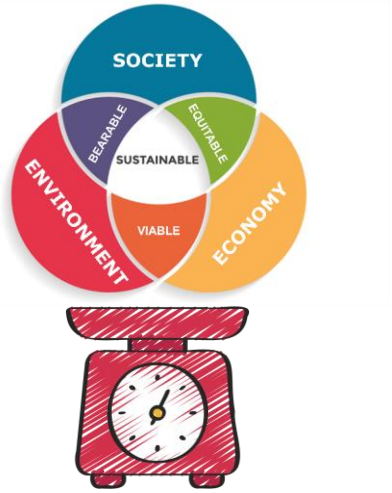
?

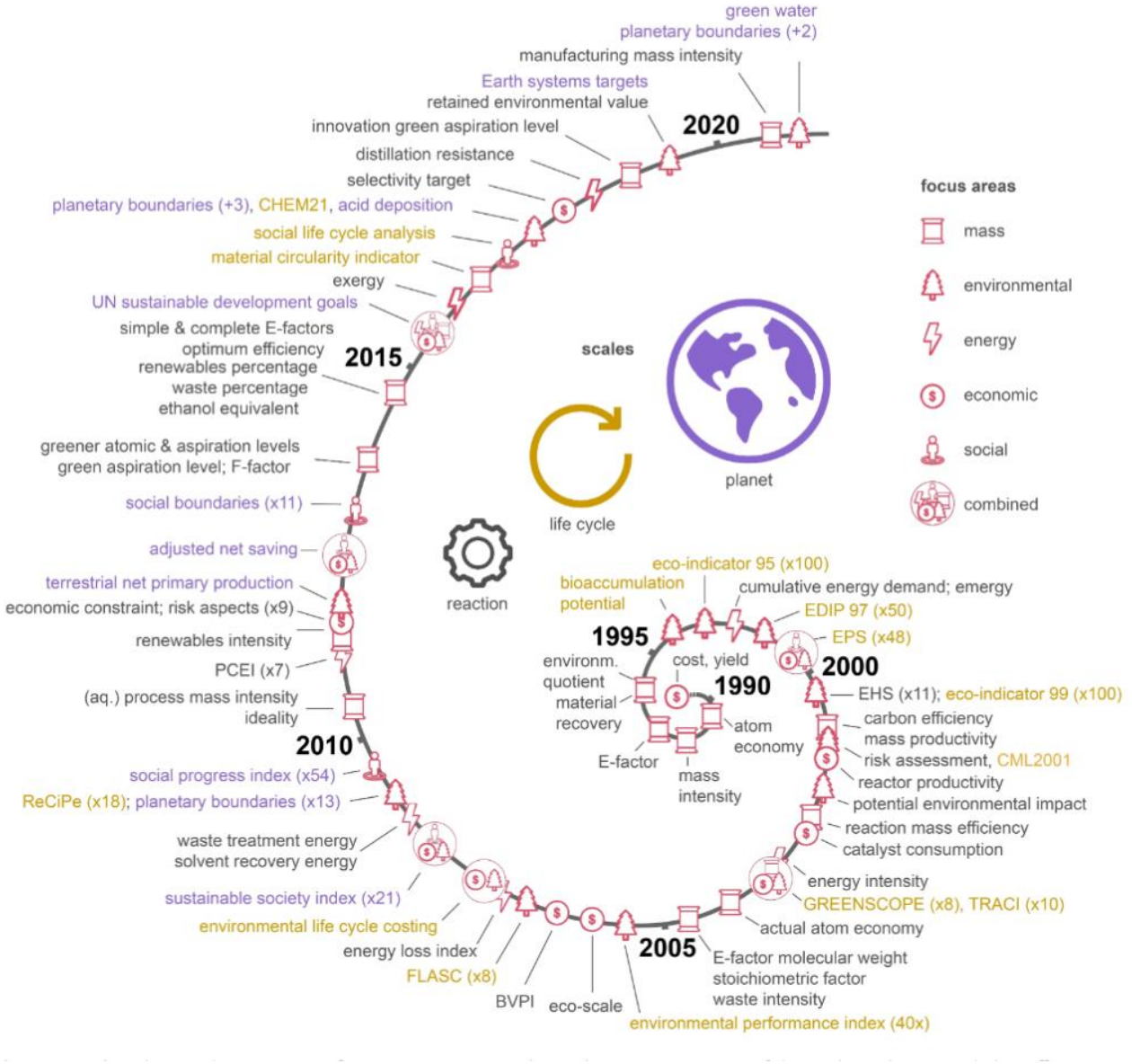
To what extent can existing and emerging technologies contribute to sustainable chemicals production?

1~2.7 Gt CO_2eq/yr

One Earth **2021**, 4, 565-583
PNAS **2019**, 116, 11187-11194

Environmental sustainability metrics for chemical systems





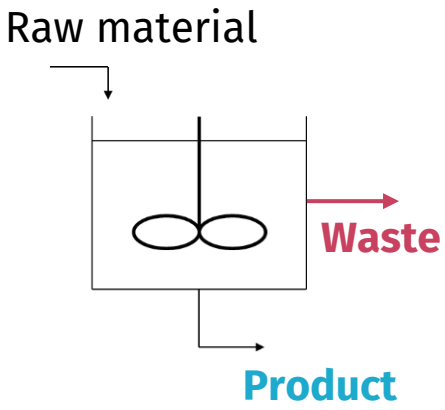
- Reaction (process level)
- Life cycle (supply chain)
- Planet (Earth)

Angew. Chem. **2024**, e202318676

How to quantify sustainability performance?

- Simple **process level metrics (reaction)**: E-Factor = **Waste (kg)**/**Product (kg)**

Easy to apply but less accurate



- **Life cycle assessment:** Covers the whole life cycle (cradle to grave, impacts on **human health, ecosystems and resources**)

Broader scope but data intensive

Chem. Ind. **1992**, 903–906
International Standard Organization ISO-14040 **1997**

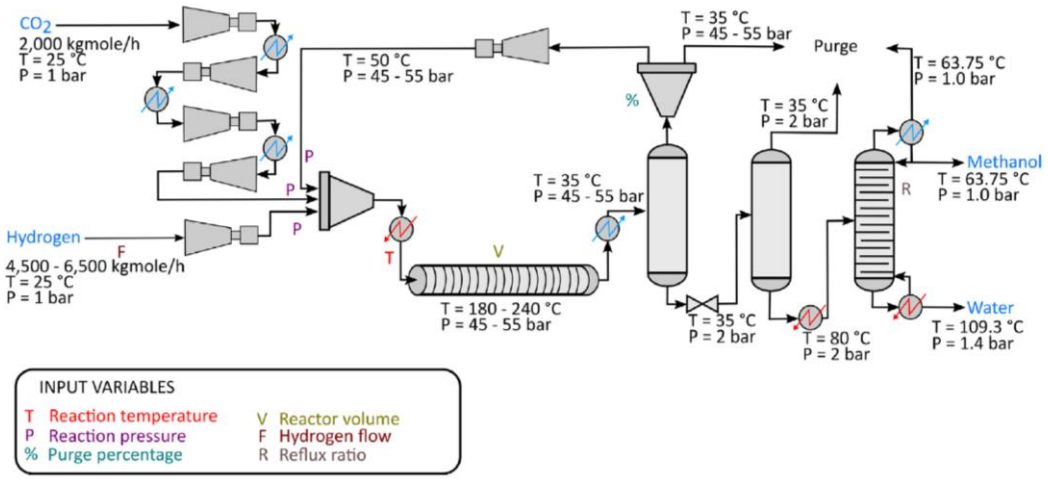
How to quantify sustainability performance?

- **Life cycle assessment**: **Combine process simulation/measurements with environmental databases**

Chemical reaction

$CO_2 + 3H_2 \rightarrow CH_3OH + H_2O$

Process simulation/measurements



Electricity

Heat

Reactants
X kg CO_2
Y kg H_2

Direct emissions

ecoinvent

Emissions per unit of flow

Fossil MeOH: **0.723 kgCO_2eq/kg**

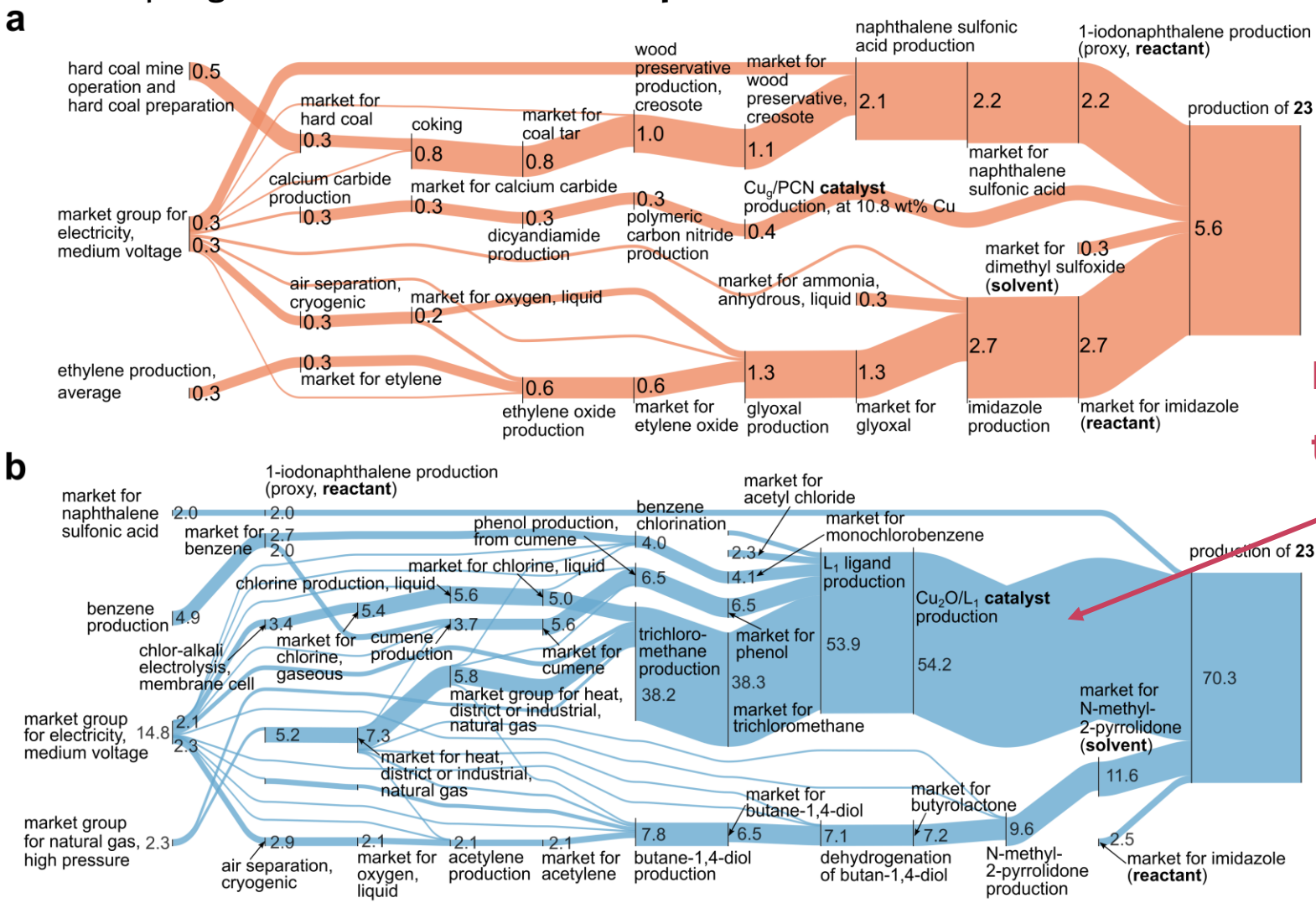
Green MeOH (H_2 from wind electrolysis, CO_2 from DAC): **-0.681 kgCO_2eq**

Energy & Environmental Science **2019**, 12, 3425-3436
Chemical Engineering Science **2021**, 246, 116891

Homogenous vs. heterogenous (Geminal-atom for cross-coupling)

Heterogeneously vs. **homogeneously** catalysed **C–N coupling**:

- Cug/PCN or Cu_2O + L1 (L1 = 4,7-dimethoxy-1,10-phenanthroline) in the synthesis of **1-(naphthalen-1-yl)-1H-imidazole** through the coupling of **imidazole and 1-iodonaphthalene**.



5.6 kg CO_2-eq/kg

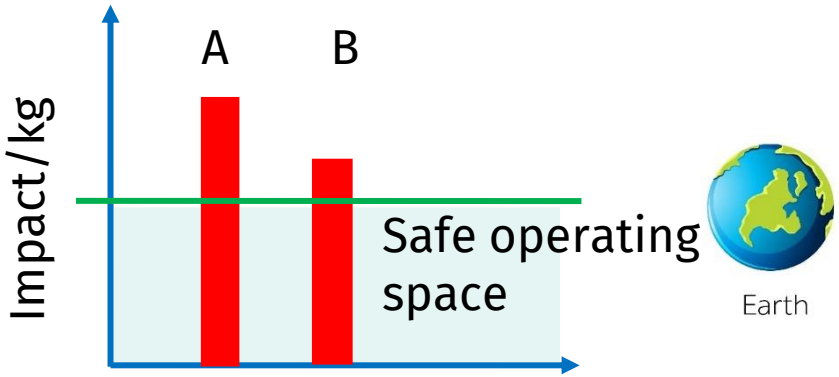
Heterogenous system avoids the use of impactful ligand

Nature **2023**, 622 (7984), 754-760

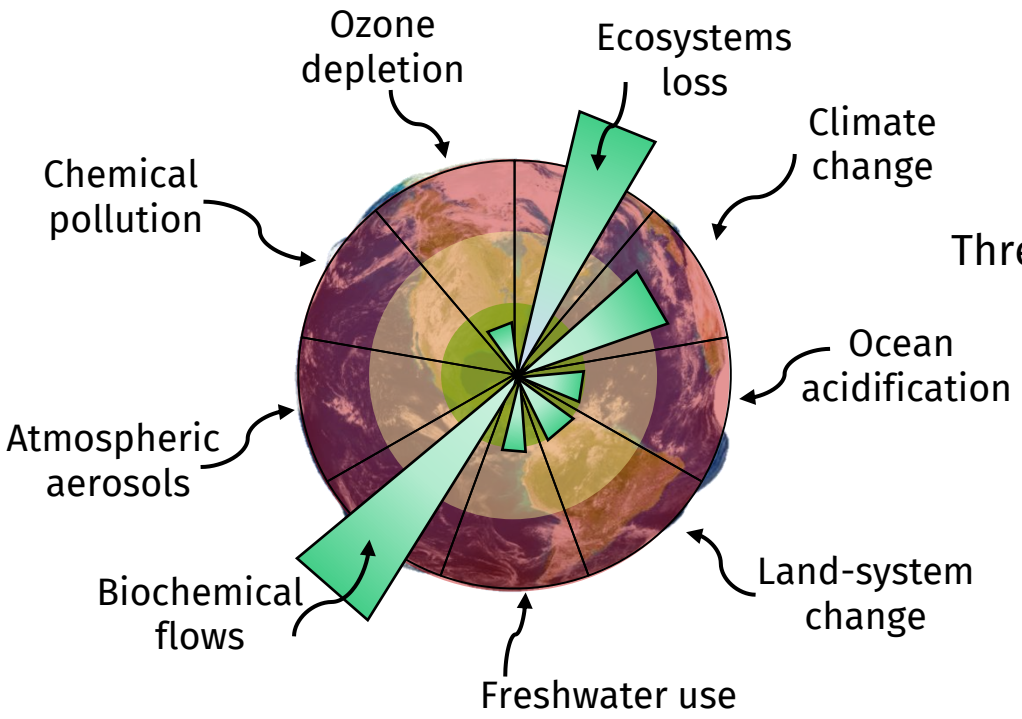
70.3 kg CO_2-eq/kg

Planetary boundaries

Current LCA standard metrics hard to interpret



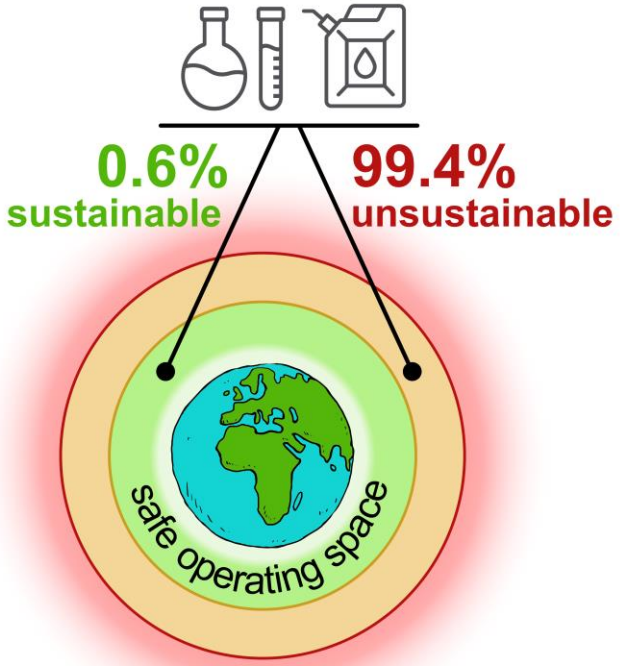
Planetary boundaries (PBs) on nine **Earth-system processes** key for resilience



Three impact levels:

- Safe op. space (SOS)
- Uncertain zone
- High-risk zone

6 PBs already transgressed!



Nature **2009**, 461, 472-475

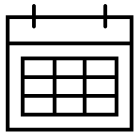
Science Advances **2023**, 9, 1-16

Green Chemistry **2011**, 23, 9881-9893

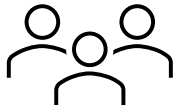
Data and sustainability: Insights from ecoinvent

ecoinvent and digital sustainability

Independent, mission-driven, not-for-profit association



Launched 20 years ago by leading Swiss research institutions



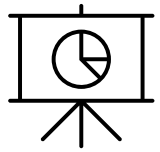
Team of 60+ experts

ecoinvent publishes and maintains a comprehensive life cycle inventory database that provides reliable and transparent information on the environmental impacts of various products and services.

Our mission

Promote and support the availability of high-quality data

Compile and review the best available data



Publish data in a regularly maintained, transparent database and support users' needs

We collect, manage, and publish background data for all kinds of environmental sustainability studies.

Connected to the LCA data ecosystem

Regular licenses

Direct data consumption or in LCA software

Managed databases

Hosting sectorial databases

Underpinning other databases

TOTEM, CarbonMinds.

Agrifoodprint

Supporting national databases

Canada, Brazil, Agribalyse

In tools and business applications (examples)

Makersite Terrascope

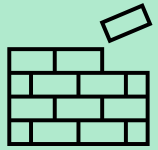
For policies and regulations

Data provider for EC's PEF/OEF initiative

ecoinvent database

Over 21,000 processes (2023) covering all regions of the world.

agricultural processes



construction materials

electricity supply

transport

wood products

chemical production

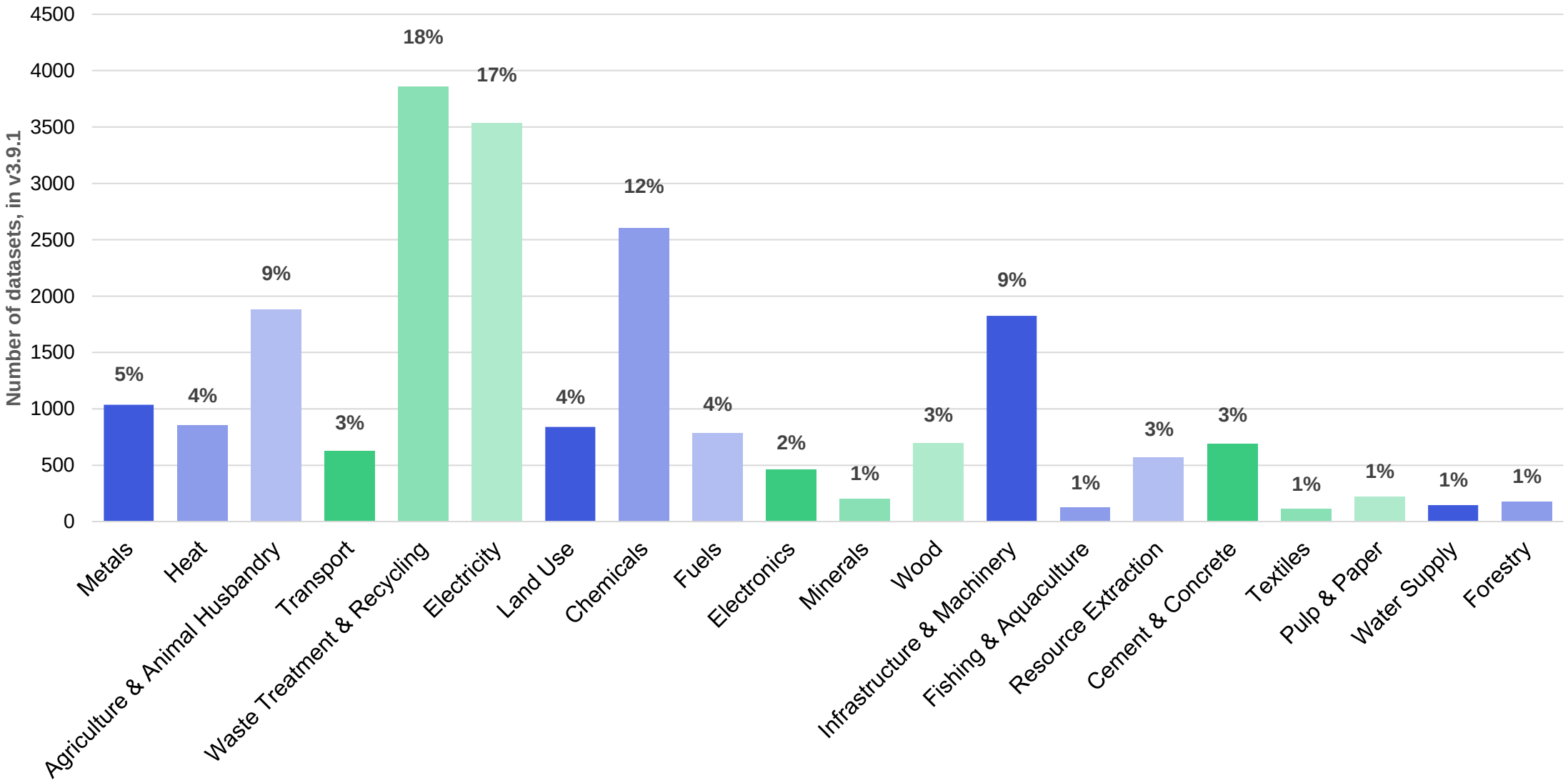
end-of-life processes

resources extraction

machinery

metal products

Database sectorial coverage



Data providers of ecoinvent

Academy

Brazilian Agricultural Research Corporation (Embrapa)

ifeu gGmbH

Paul Scherrer Institut (PSI)

Swiss Federal Institute of Technology Zurich ETH

University of Cape Town

Industry

Paper and carton: CEPI, ECMA, EPIS, Eurosac, Pro-Carton

Textile: Cotton Incorporated

Metals: IZA, IAI, EAA, CI

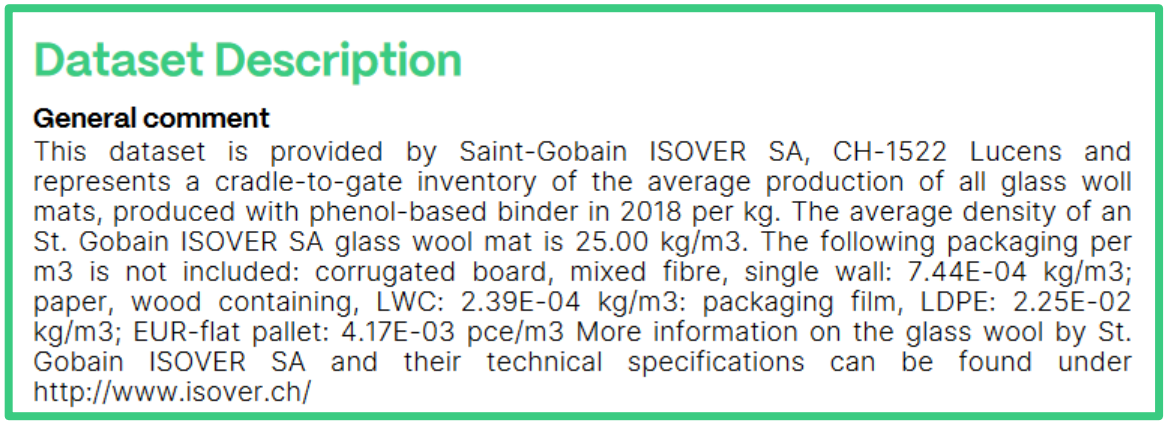
Chemicals: EUROPUR; Fertilizers Europe, Plastics Europe, Yara

Construction: **Saint-Gobain**, CemSuisse

National initiatives

Some regional/national database initiatives integrate their national data fully within our database:

- Brazil
- Quebec



Dataset Description

General comment

This dataset is provided by Saint-Gobain ISOVER SA, CH-1522 Lucens and represents a cradle-to-gate inventory of the average production of all glass woll mats, produced with phenol-based binder in 2018 per kg. The average density of an St. Gobain ISOVER SA glass wool mat is 25.00 kg/m3. The following packaging per m3 is not included: corrugated board, mixed fibre, single wall: 7.44E-04 kg/m3; paper, wood containing, LWC: 2.39E-04 kg/m3: packaging film, LDPE: 2.25E-02 kg/m3; EUR-flat pallet: 4.17E-03 pce/m3 More information on the glass wool by St. Gobain ISOVER SA and their technical specifications can be found under http://www.isover.ch/

Initiative

HiQ-LCA: ecoinvent is the project partner leading data management

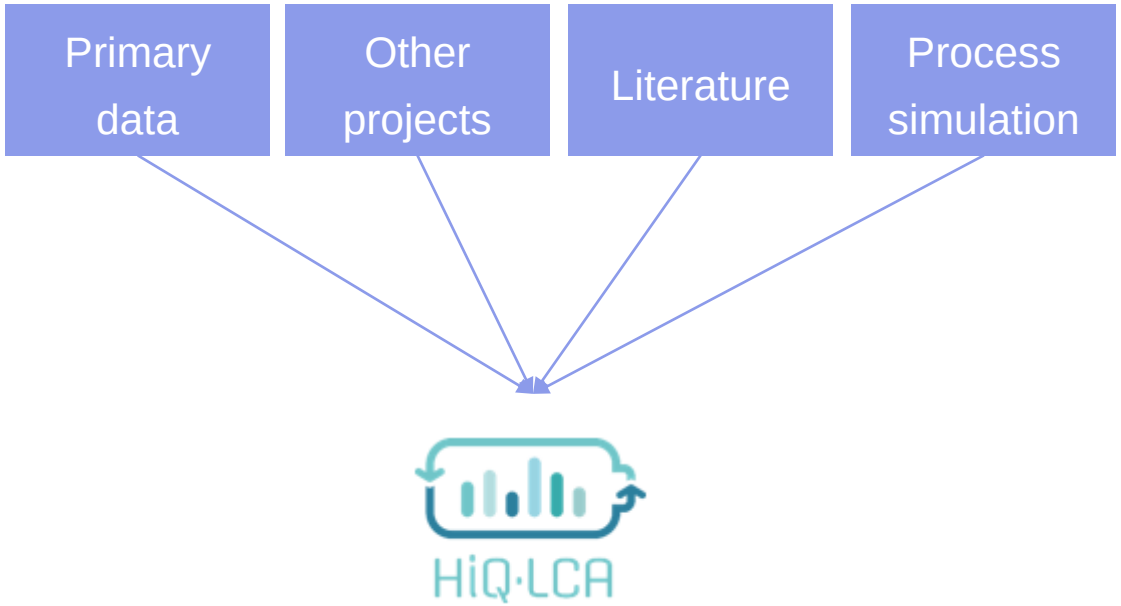
Create detailed, representative, reliable and transparent LCA datasets for batteries

- Website: https://hiq-lca.eu/

This project receives funding from

eit RawMaterials Connecting matters

Co-funded by the European Union



Database maintenance

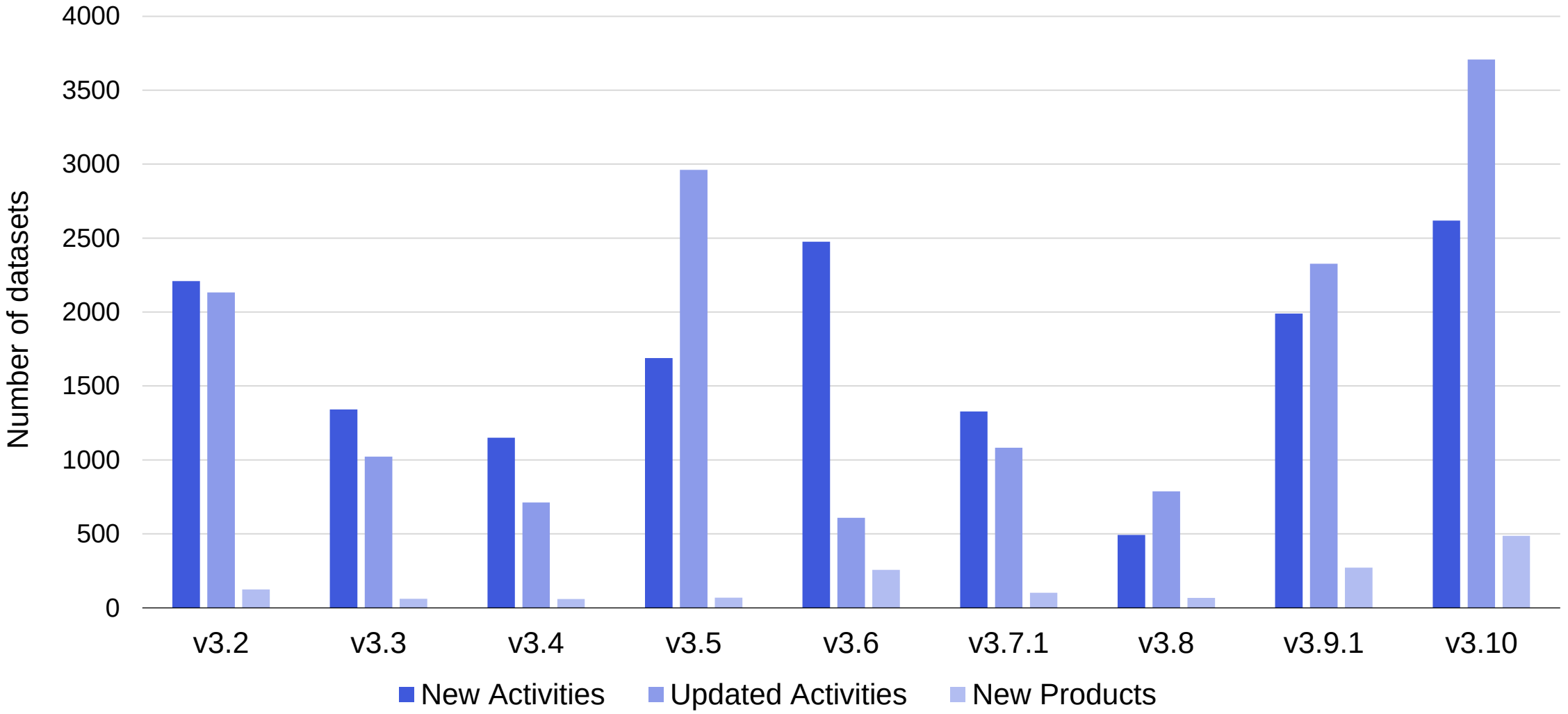
By maintaining the database, guidance from sustainability assessment becomes more effective.

Maintenance means:

- Constant correction of bugs and errors.
- Frequent update of fast-evolving data (i.e., electricity mixes).
- Update of data as they grow old.
- Update of data as new features are added.
- Addition of new data (new technologies, new regions).

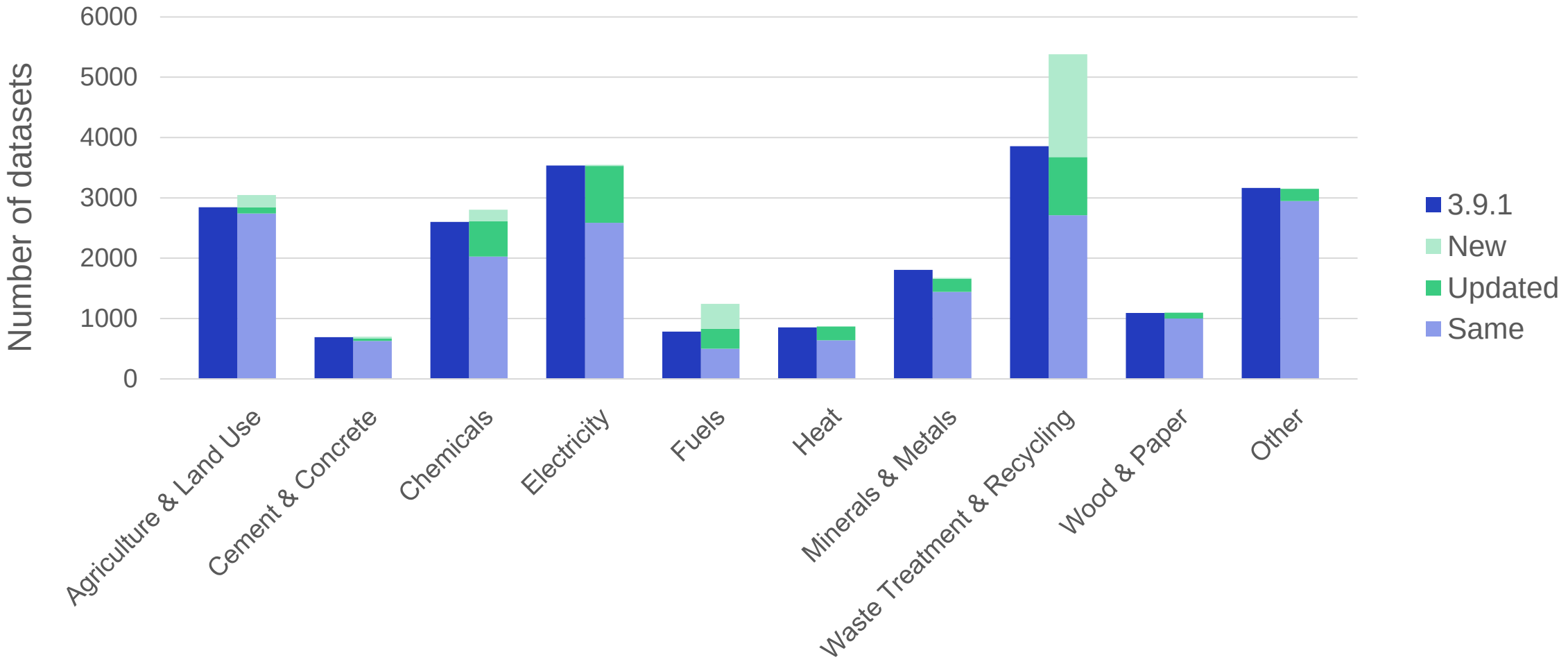
These maintenance principles are equally vital for digital sustainability tools developed by PSE!

The database over the years



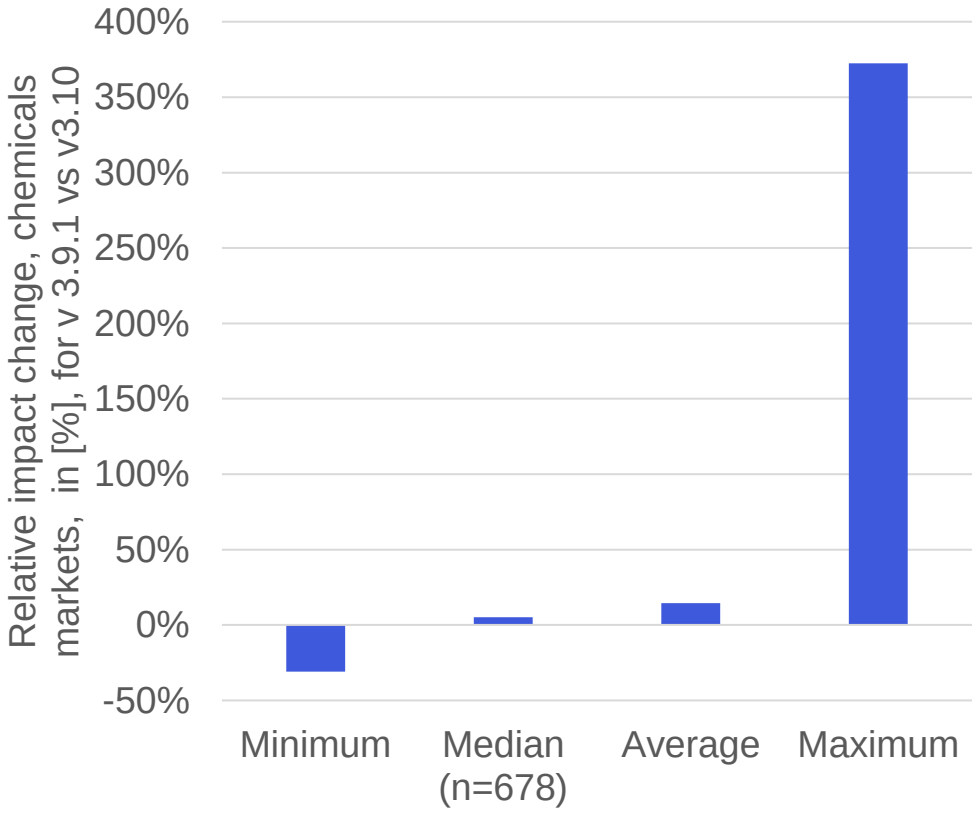
Numbers for Allocation, cut-off

Number of datasets in 3.9.1 and 3.10

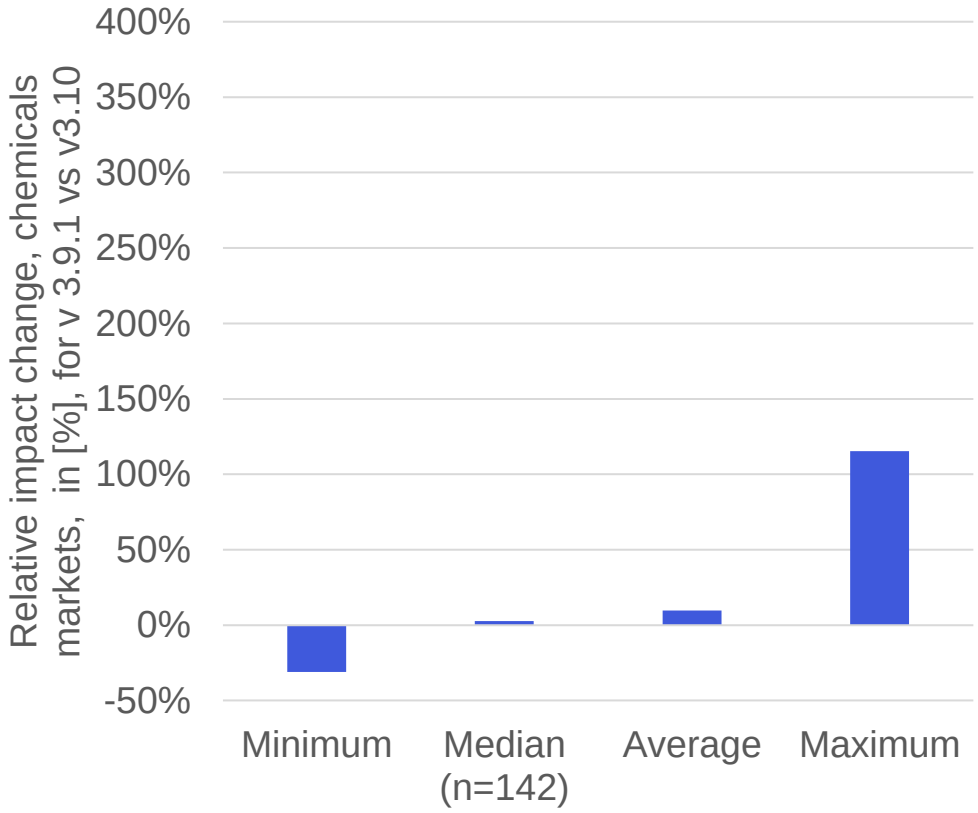


3.10: GWP change for chemicals

All chemical market activities



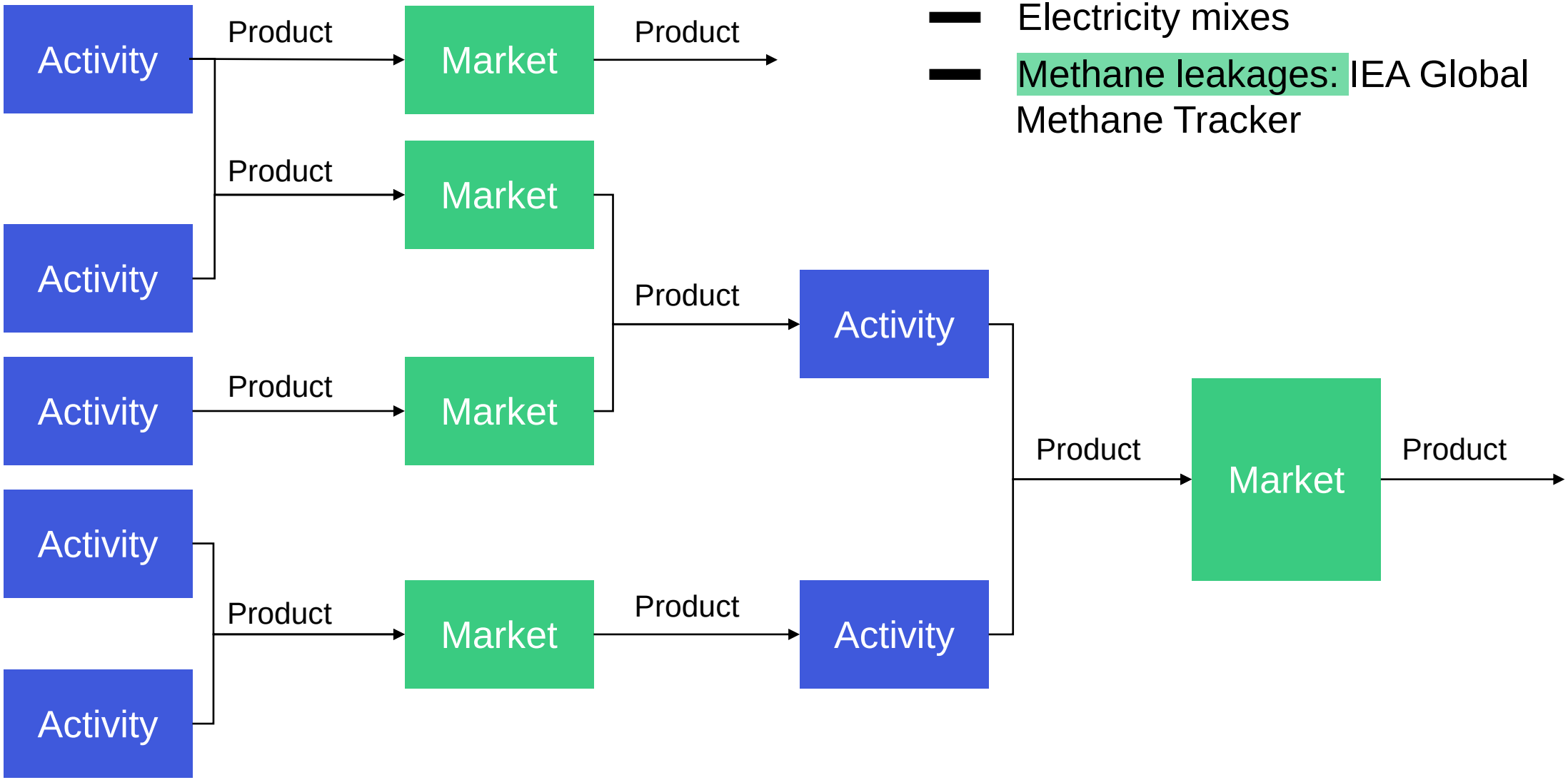
European chemicals market activities



Use of outdated data may lead to less accurate assessments aimed for informed decision-making.

Why did environmental impacts change after a release?

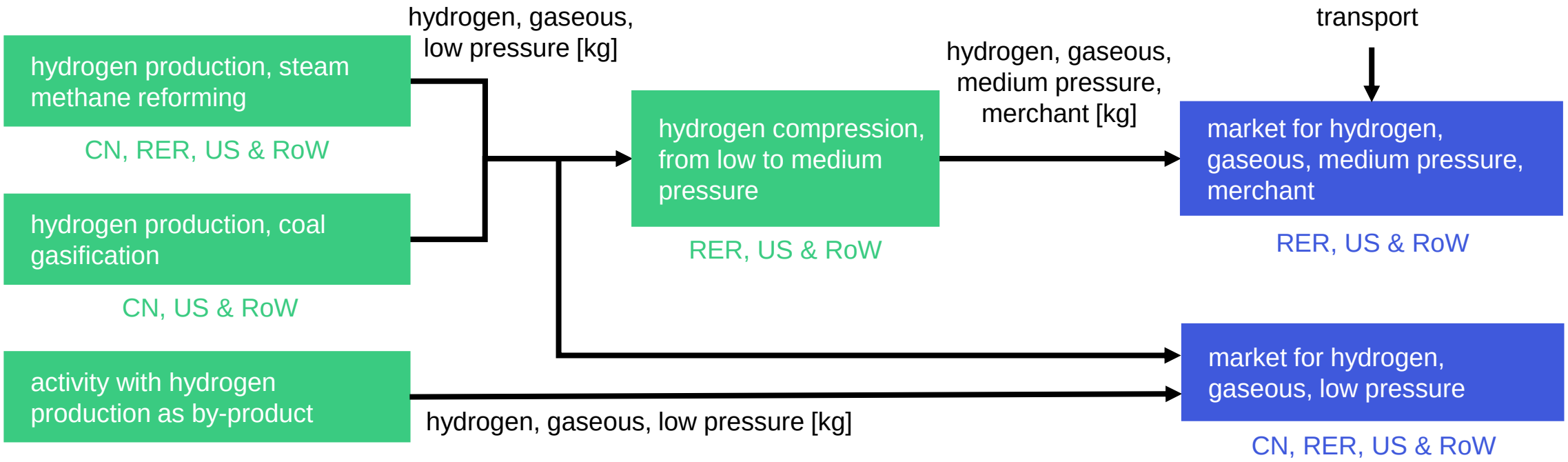
Linking: calculating the database



Hydrogen supply chain

- New and upaded activities
  - coal gasification & steam methane reforming (hydrogen is the **reference product**)
- Updated activities
  - steam cracker & chlor-alkali electrolysis (hydrogen is **a by-product**)

- Significant increase in impact scores in 3.10 vs 3.9.1 since coal gasification was not previously covered.



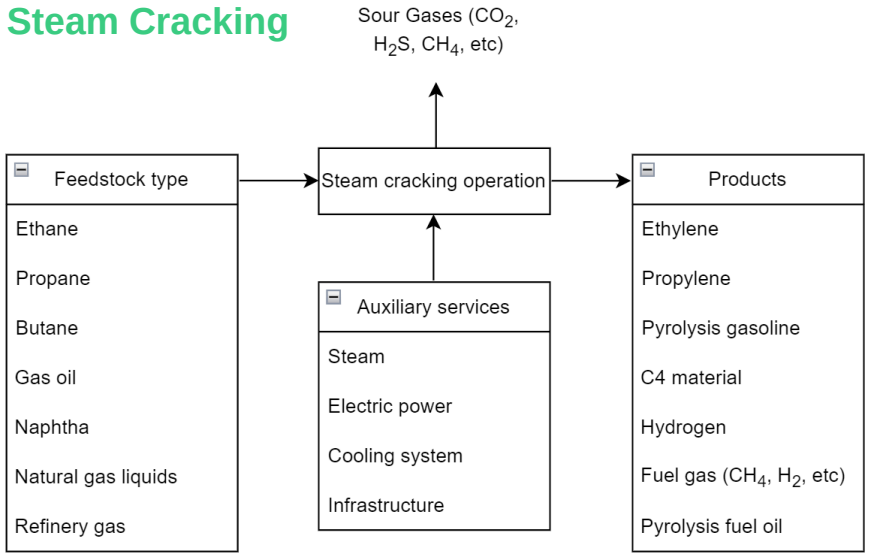
Key petrochemicals production

- Replaced industry-based aggregated steam cracking data with more recent and transparent ones.
- Updated the data for key chemical precursors and their derivatives.

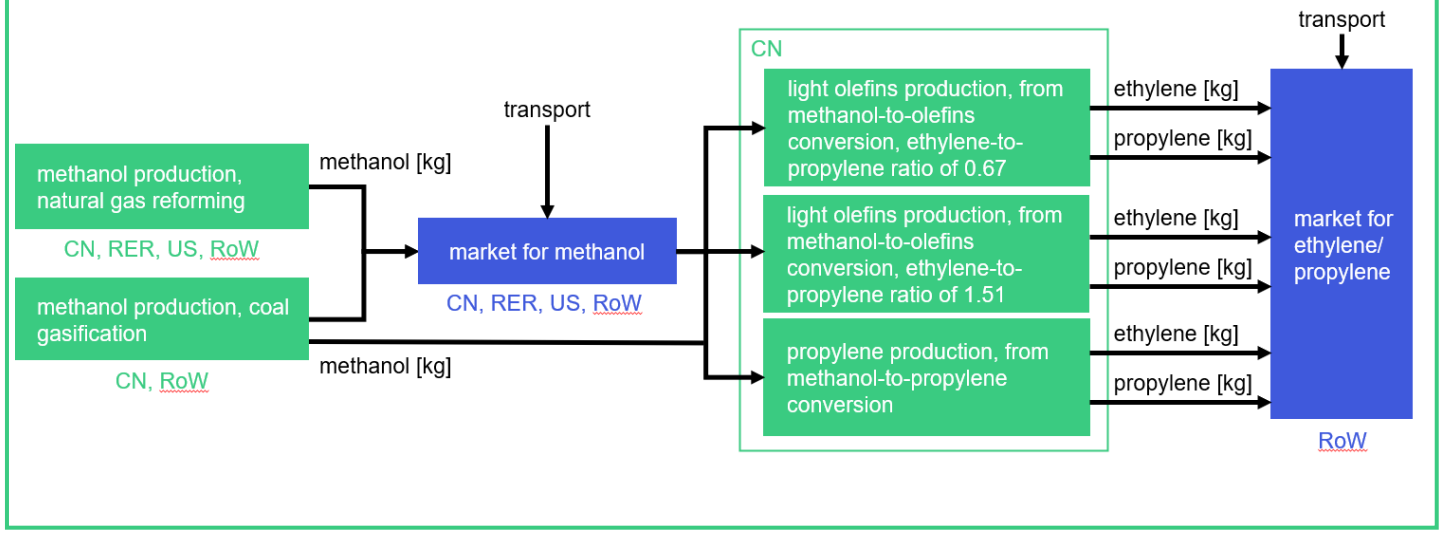
ifeu INSTITUT FÜR ENERGIE- UND UMWELTFORSCHUNG HEIDELBERG

PLASTICS EUROPE Enabling a sustainable future

Steam Cracking



Methanol production, and derivatives

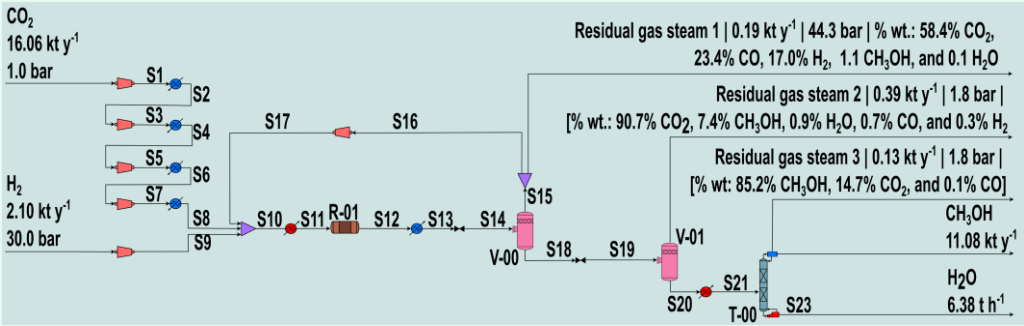


PSE and digital sustainability

PSE principles have the potential to pave the way toward a sustainable future by guiding decision-making.

Main challenge: Digital enabled sustainability is data-intensive!

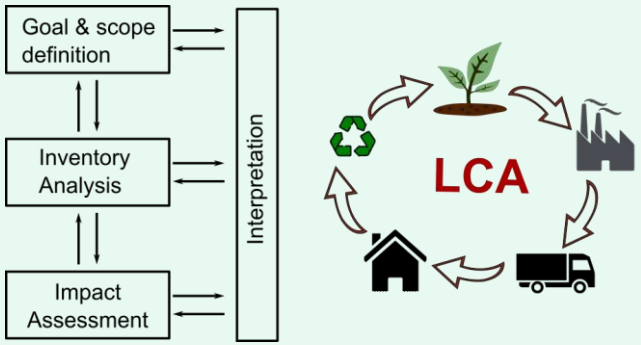
Process modeling



Mathematical Programming

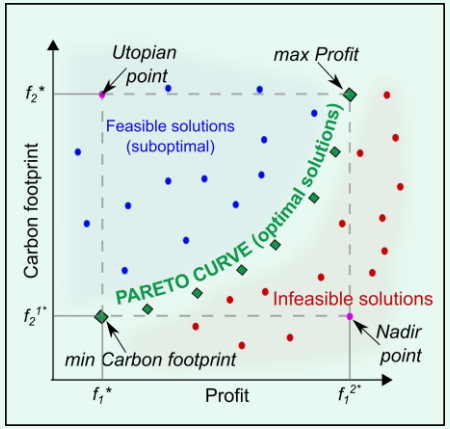
$$\begin{aligned} min \quad & f(x,y) \\ s.t. \quad & h(x,y) = 0 \\ & g(x,y) \leq 0 \\ & x \in \Re^n \\ & y \in \{0,1\}^m \end{aligned}$$

Life cycle assessment (LCA)



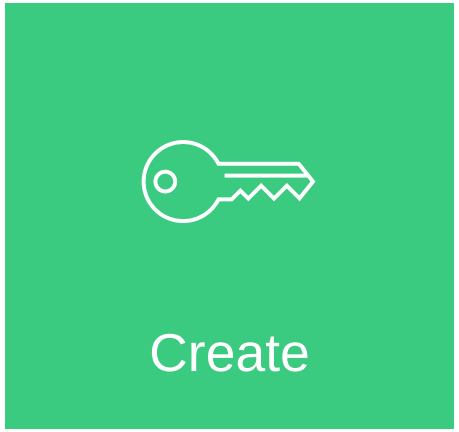
Multi-objective optimization: Life cycle optimization (LCO)

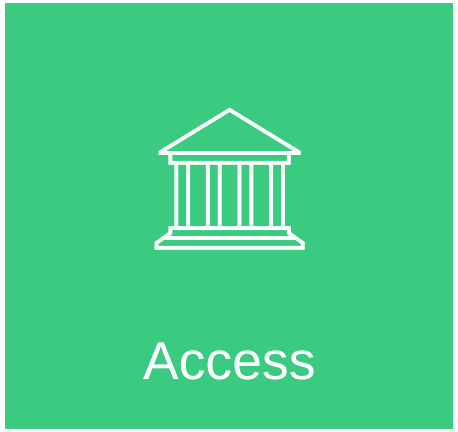
$$\begin{aligned} min \quad & f_1(x,y), \dots, f_k(x,y) \\ s.t. \quad & h(x,y) = 0 \\ & g(x,y) \leq 0 \\ & x \in \Re^n, y \in \{0,1\}^m \end{aligned}$$

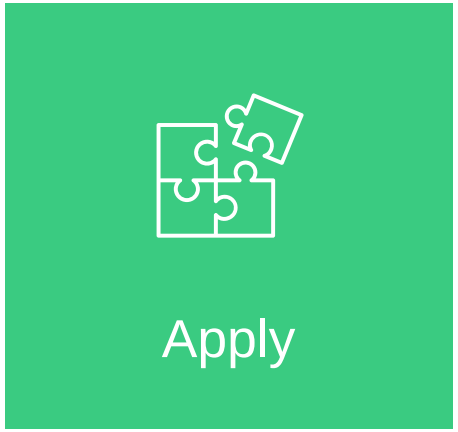


Ioannou, Iasonas (2023). Doctoral Dissertation, ETH Zurich

Data and PSE



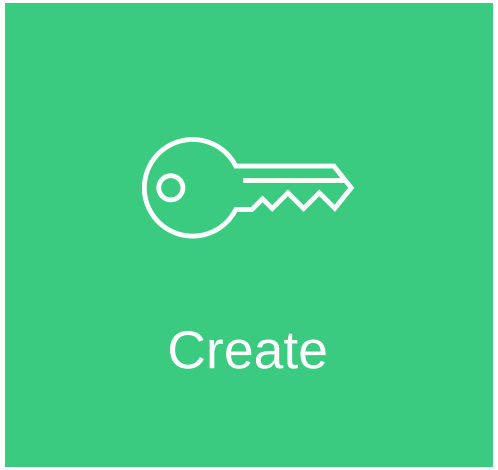




The PSE community could

- satisfy at scale the ever-increasing demand for data creation.
- improve the accessibility to process data and digital tools.
- apply effectively sustainability data in tools to facilitate holistic environmental assessments and sustainable decision-making.

Data and PSE



PSE tools have pioneered the creation of sustainability data for chemical processes, from machine learning to process modelling and optimization algorithms!

- Tools designed to simplify early-stage assessments.
- Streamlined process simulation for chemicals manufacturing.
- Early assessment for potential designs of integrated biorefineries.
- Predictive assessments for chemical processes using machine learning.

1. Minten, Vandegehuchte, Jaumard, Meys, Reinert, and Bardow (2024). https://doi.org/10.1039/D4GC00964A

2. Parvatker and Eckelman (2020). https://doi.org/10.1021/acssuschemeng.0c00439

3. Moncada, Posada, and **Ramírez** (2015). https://doi.org/10.1002/bbb.1580

4. Kleinekorte (2022). Doctoral Dissertation, RWTH Aachen University

Data and PSE

Access

The PSE community could enhance the accessibility to robust process data and tools based on first principles.

- Disclose data in publications for future reference and use.

  ➔ **vital for digital sustainability advances**
- Establish a specialized journal, "PSE Sustainability Data and Models," dedicated to publishing and hosting data and models, with thorough data review.

  ➔ **raw data need curation, e.g., ecoinvent conducts multiple review stages to ensure high quality.**
- Develop open-source tools for experts and non-experts.
- Provide data and tools in initiatives and databases for a wider use.

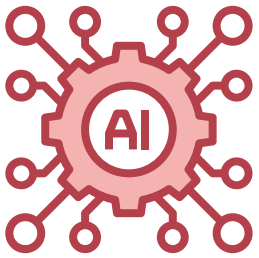
Data gaps and background data

Streamlined LCA methods for chemicals

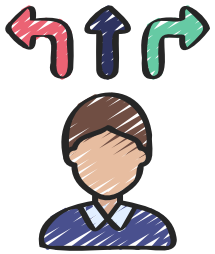
~1 Million registered chemicals

LCA data of only a few thousand chemicals

1. Impact estimates using **machine learning**



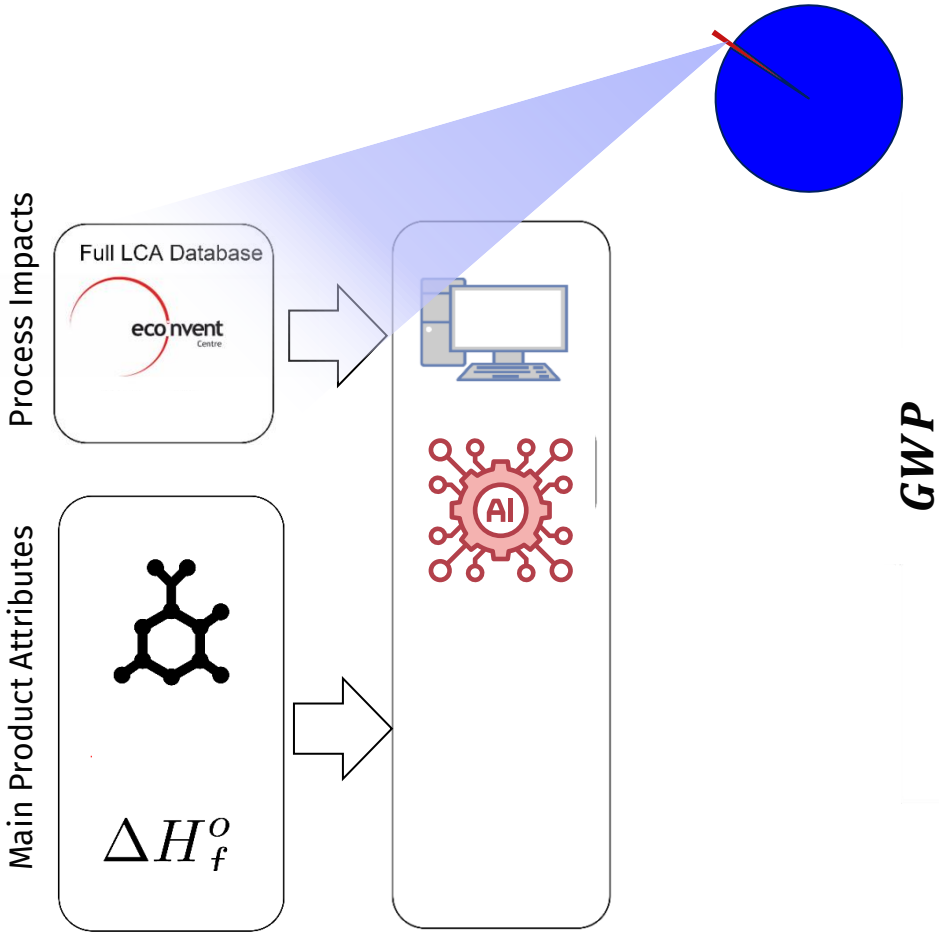
2. Impact estimates and insights using **augmented LCA data**



Avoid metal X

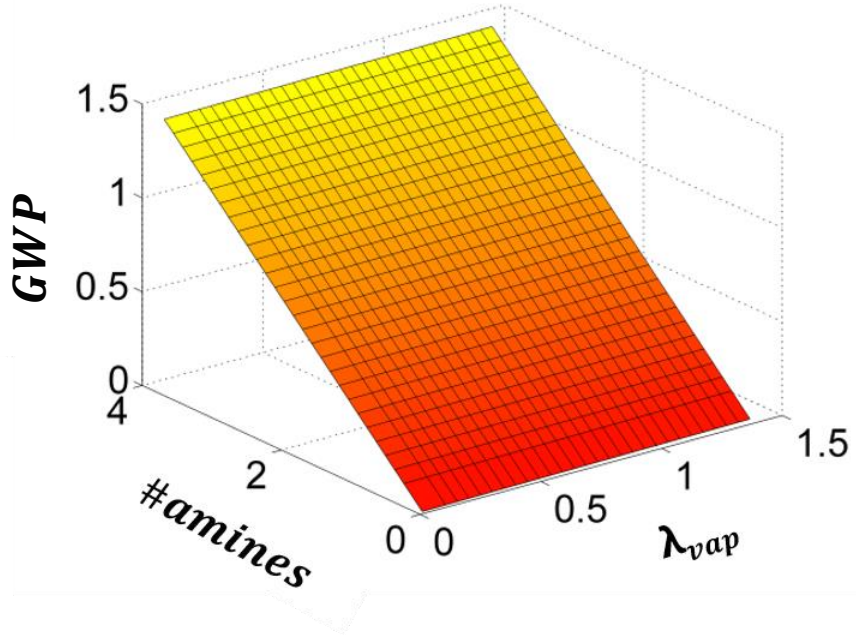
Select reaction Y over Z...

Streamlined LCA methods for chemicals: ML for impacts prediction



~1 Million registered chemicals

LCA data of only a few thousand chemicals

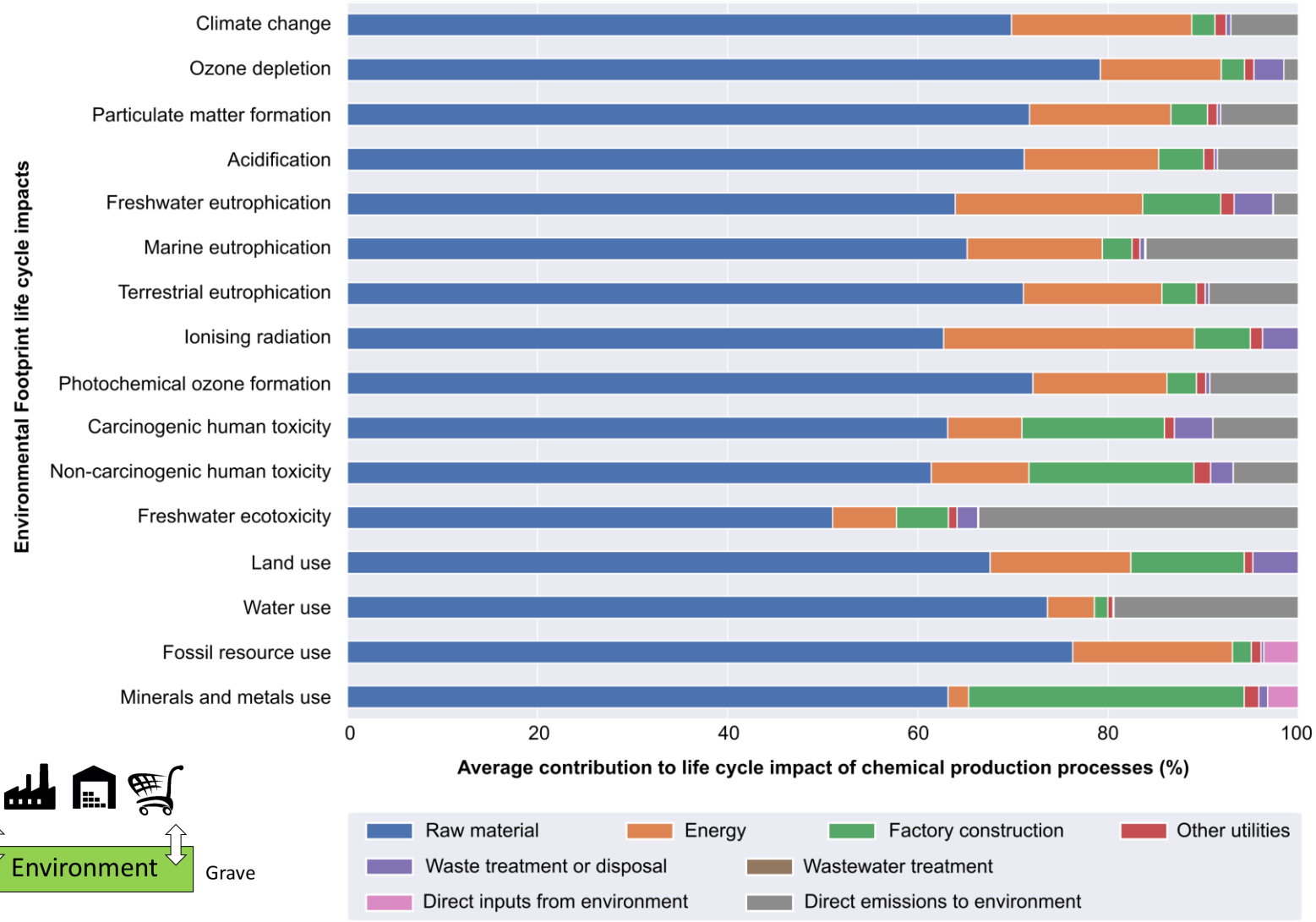


$$GWP = f(structure, \lambda_{vap})$$

Computers & Chemical Engineering **2018**, 108, 179-193

ACS Sustainable Chemistry and Engineering **2024**, 12, 2700-2708

Motivation for generating augmented LCA data: Impact breakdown



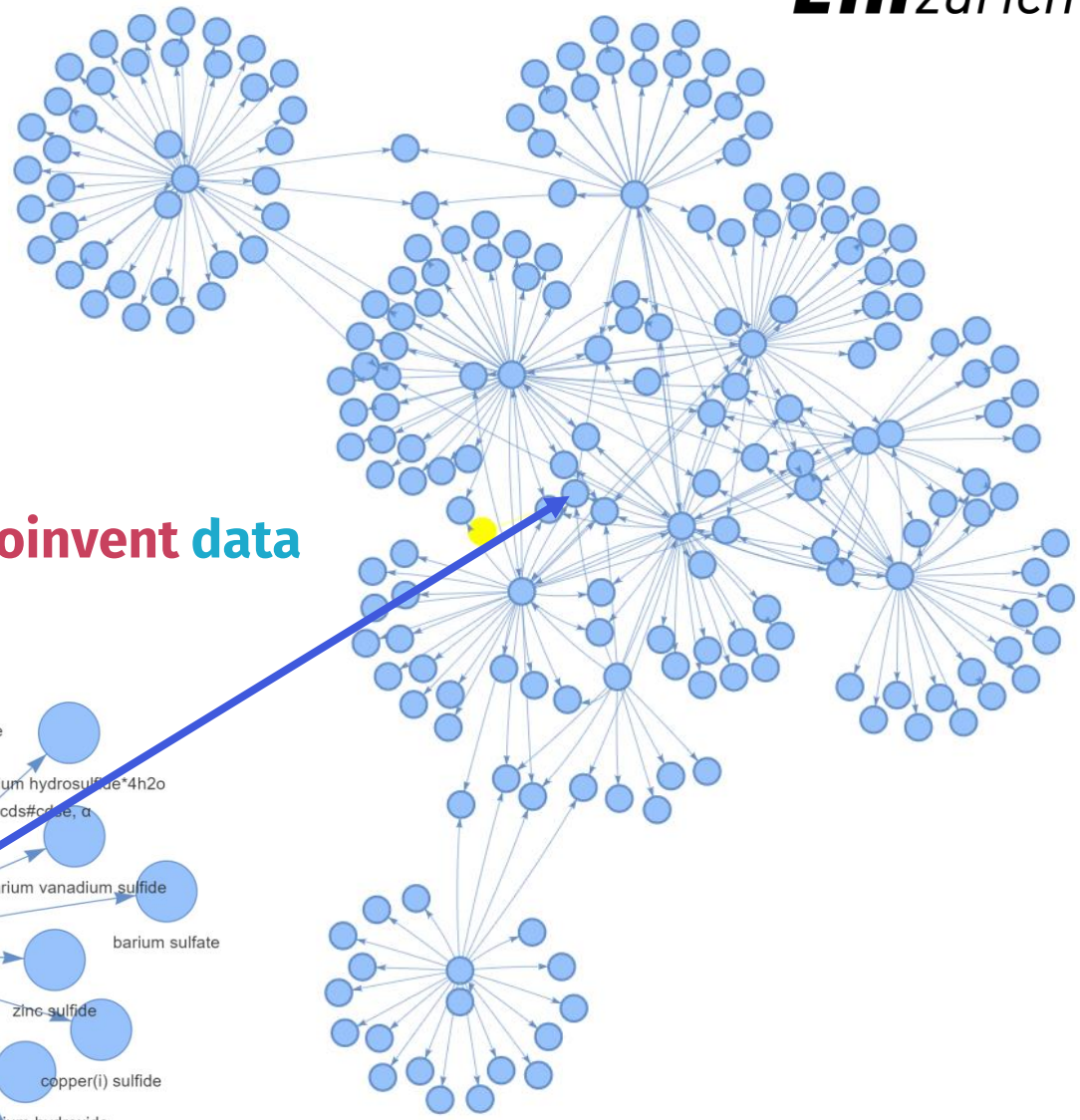
- **Average contribution highest from raw materials** (**51 - 80%** considering **~700** chemicals)

Green Chemistry ***2024***, under review

Reaxys for LCA data augmentation

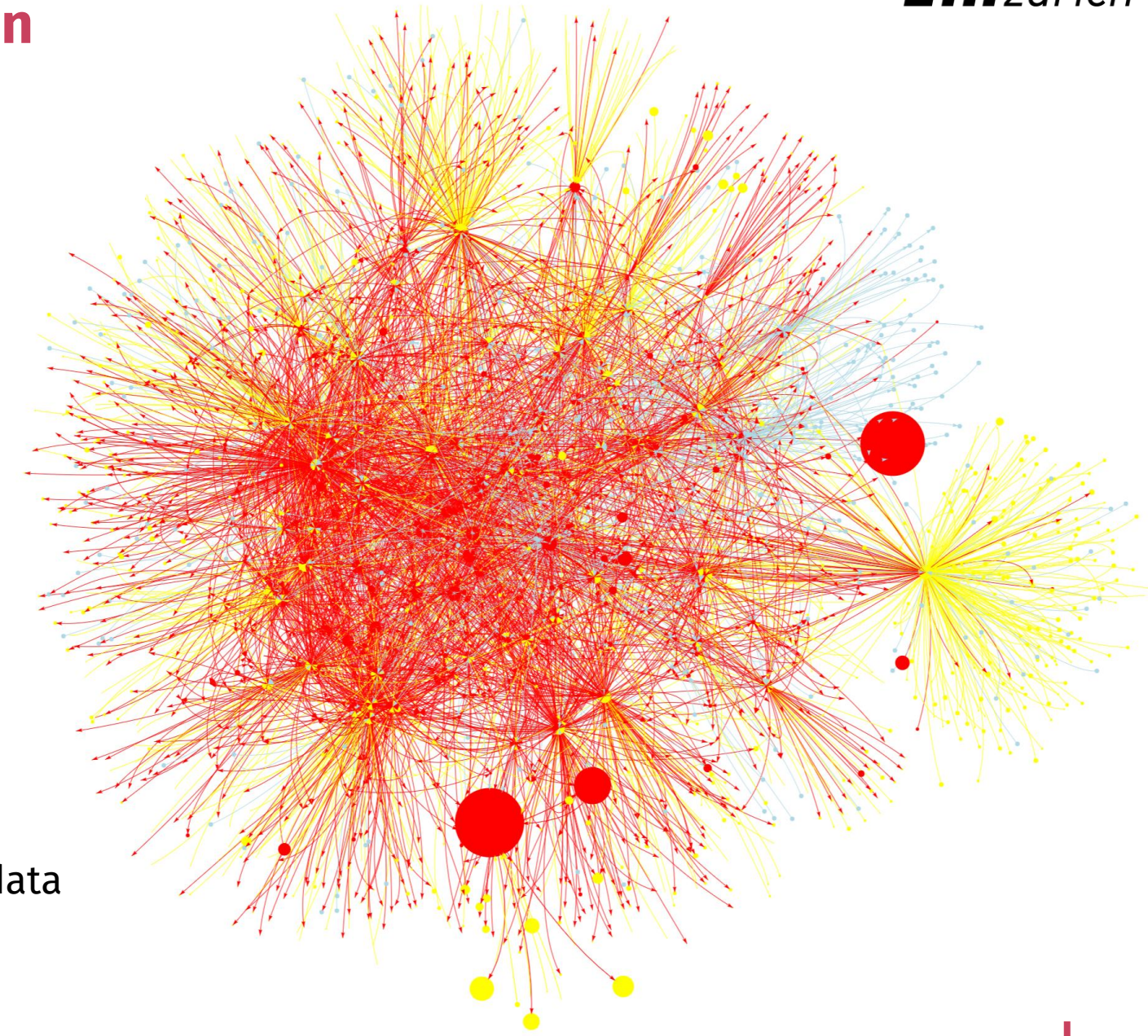
- Start from an **ecoinvent** product
- Find the **chemical neighborhood**
- **Repeat** the same procedure
- Determine unknown impacts from **stoichiometric and ecoinvent data**

$$\begin{aligned} \min_x \quad & f(x) \\ \text{s.t.} \quad & h(x) = 0 \\ & g(x) \leq 0 \end{aligned}$$



Reaxys for LCA data augmentation

- **Chemicals from ecoinvent (171)**
- **Estimated chemicals (1752)**
- **Other chemicals (147)**

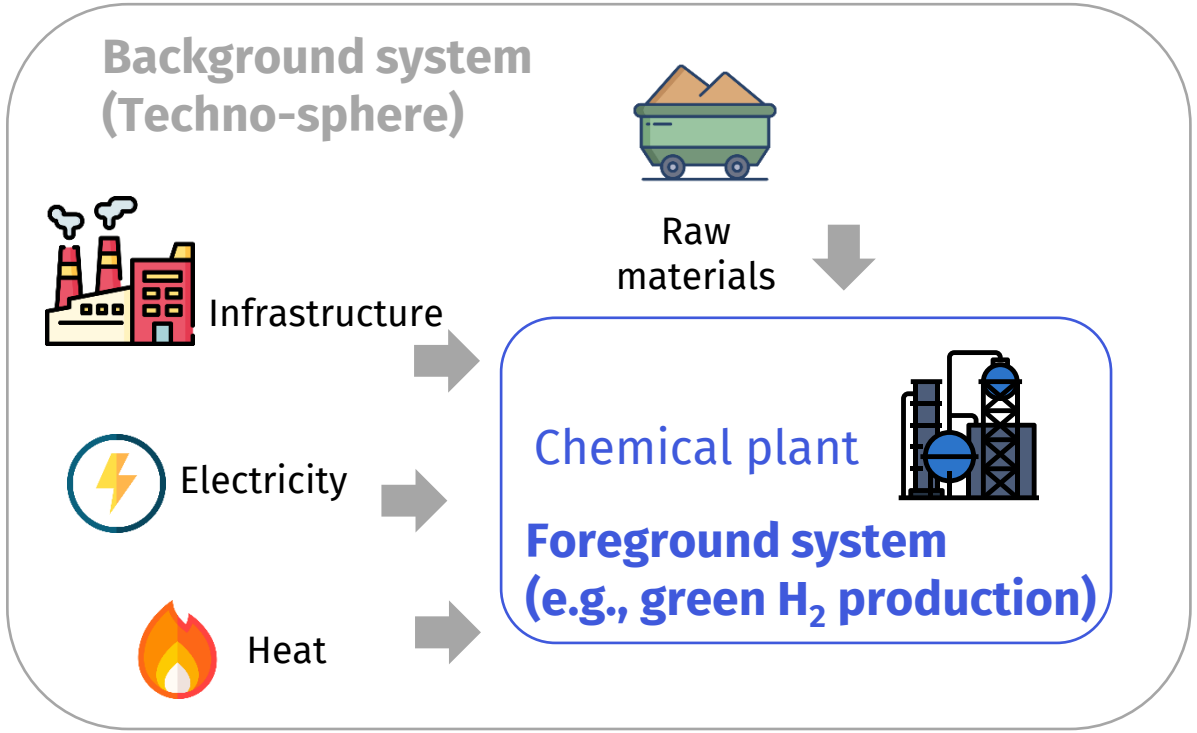


Augmented ecoinvent

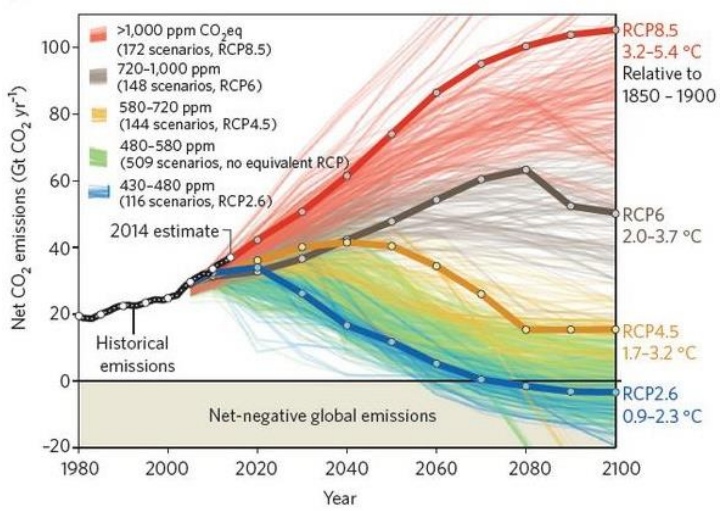
Challenges:

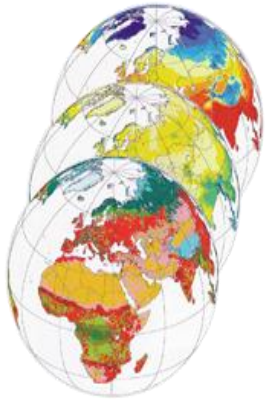
- Missing reactants/products/stoichiometric data
- Alternative pathways for the same molecule
- No energy requirements

Prospective life cycle assessment

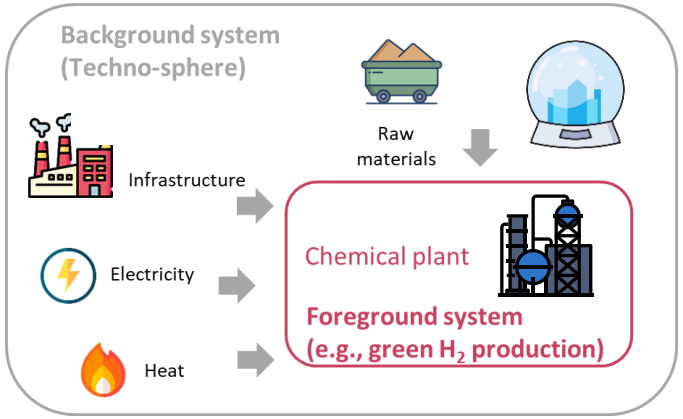


- Background system often assumed to be fixed
- However, economy is expected to change



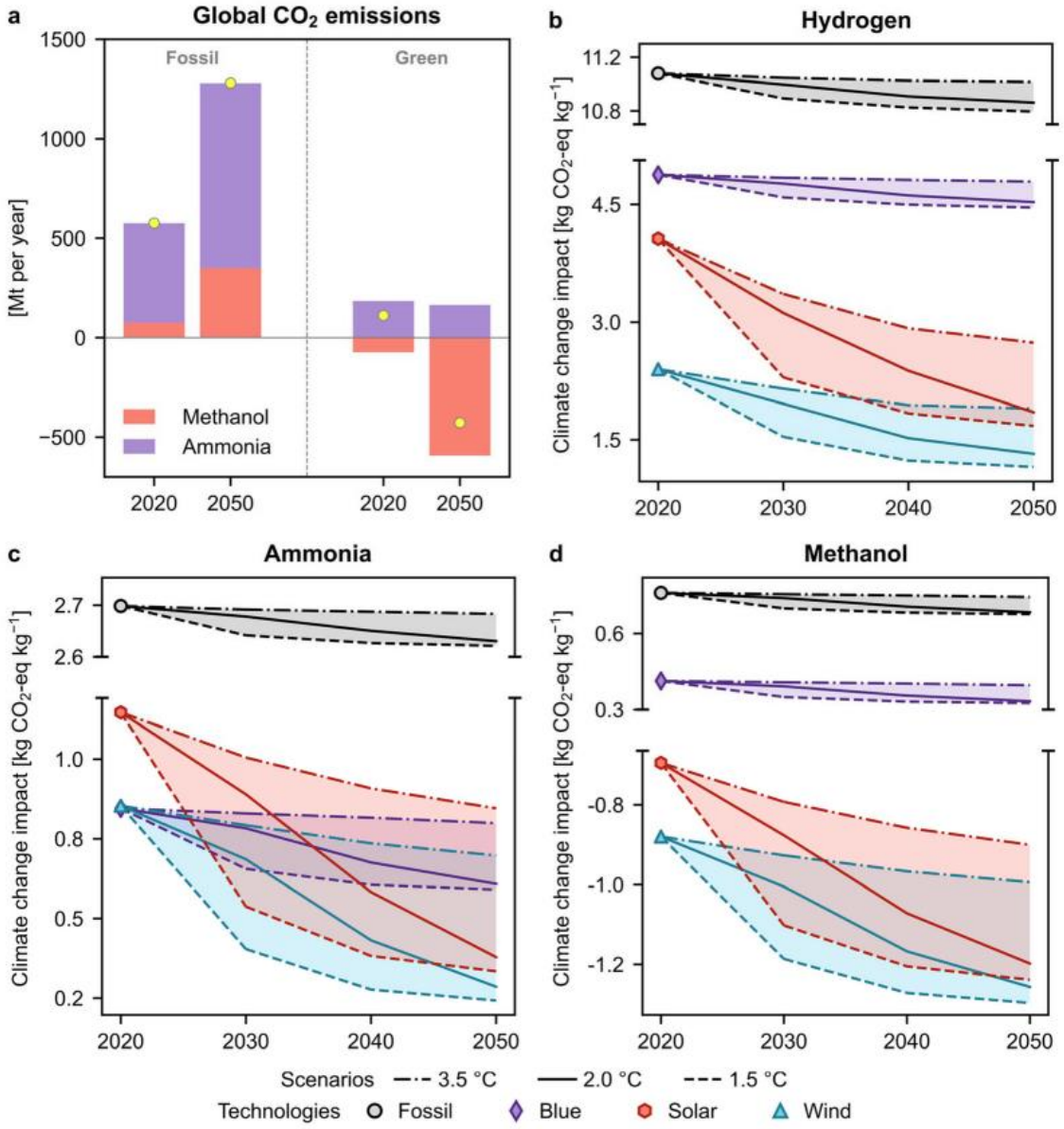


Integrated Assessment Models and socio-economic pathways



Prospective life cycle assessment based on future scenarios (*premise*)

Prospective life cycle assessment

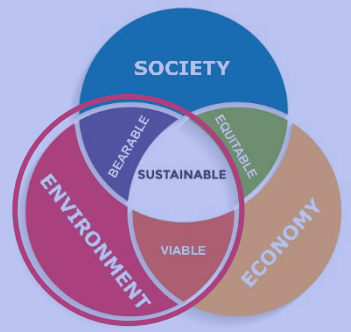


- Carbon footprint of **future green chemicals** dropping by 90% (vs. 10% in fossil routes)

Green Chemistry **2024**, accepted

Life cycle optimization

Multi-objective model based on superstructures



$$\begin{aligned} min \quad & f_1(x,y), \dots, f_k(x,y) \\ s.t. \quad & h(x,y) = 0 \\ & g(x,y) \leq 0 \\ & x \in \Re^n, y \in \{0,1\}^m \end{aligned}$$

Objective function (e.g., cost, impacts)

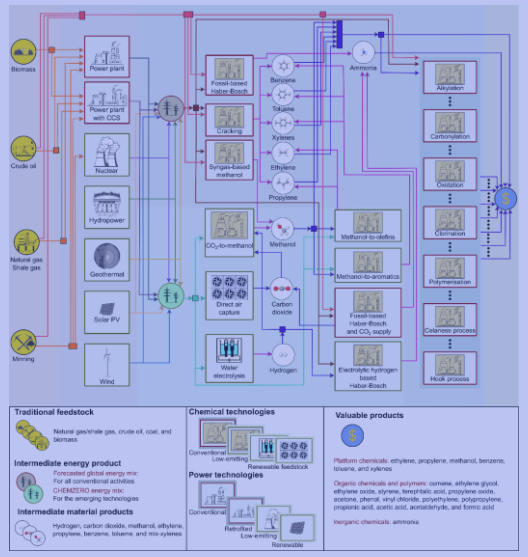
Process equations (e.g., mass balances)

Specifications

Continuous variables (e.g., pressures, flows)

Discrete variables (logic decisions)

Superstructure



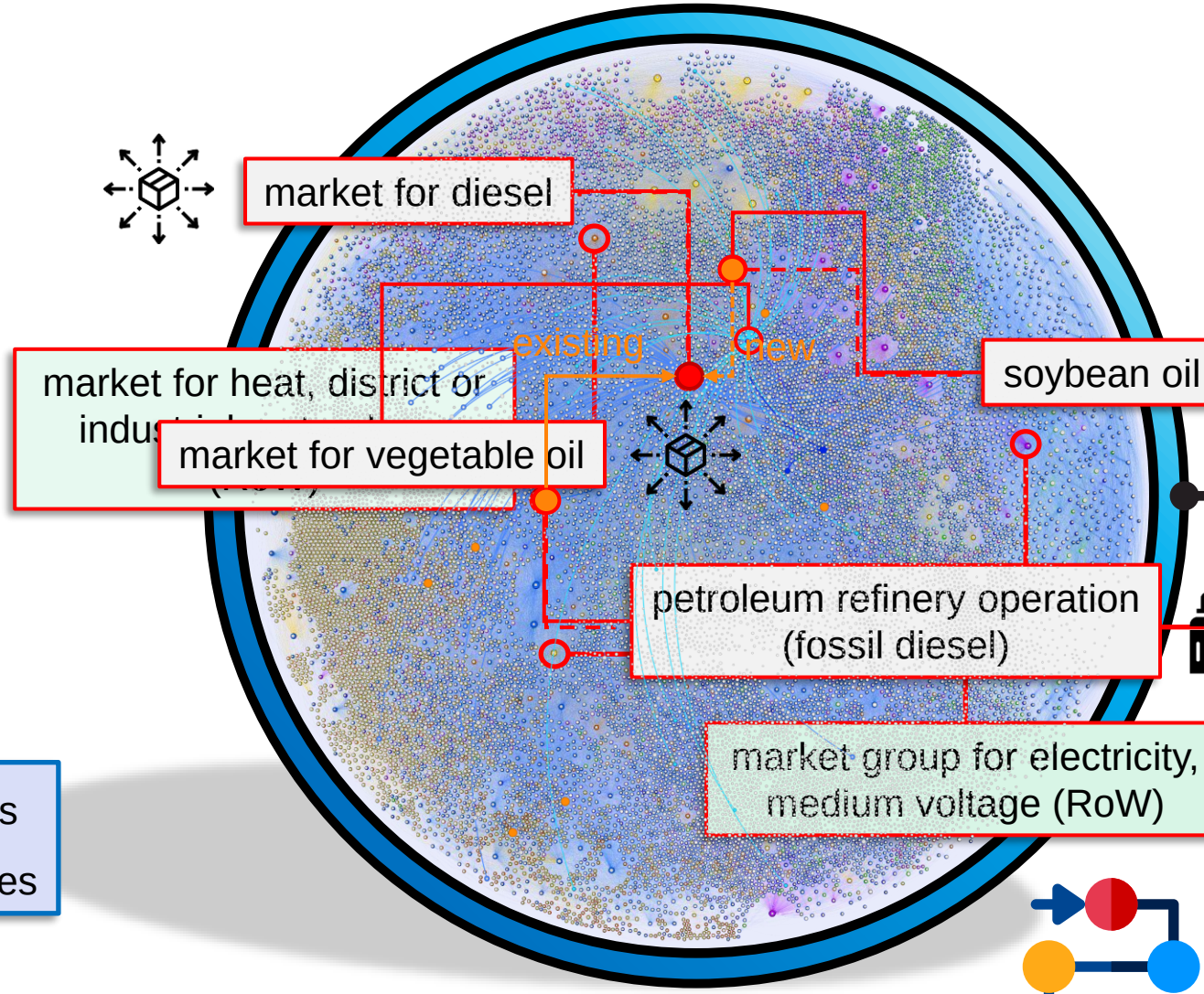
Life cycle sustainability assessment

Computers & Chemical Engineering **1999**, 23, 1509-1526
Computers & Chemical Engineering **2010**, 34, 1365-1376

Techno-sphere wide implications of emerging routes

ETH zürich

- Material
- Electricity
- Heat
- Transport
- Land use



ecoinvent 3.8

(cutoff system model)

market group for transport, freight, lorry, unspecified (GLO)

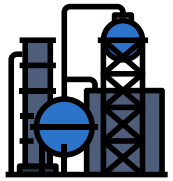
- 19.000 Nodes
- 200.000 Edges

$$\begin{aligned} min \quad & f_1(x,y), \dots, f_k(x,y) \\ s.t. \quad & h(x,y) = 0 \\ & g(x,y) \leq 0 \\ & x \in \Re^n, y \in \{0,1\}^m \end{aligned}$$

Relevant questions in Green Chemistry and beyond

- Which C feedstocks?

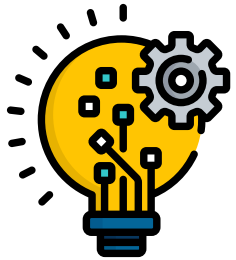
- Which renewable technologies?



- Break-even efficiency and bottlenecks?

- Where, when and how to deploy technologies?

- How to optimally couple the chemical industry with other sectors?



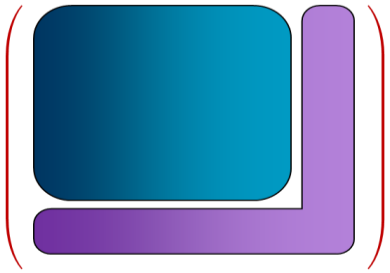
PULPO: An *oracle* to underpin *sustainable* technology development...

User Input

(processes)

1. functional unit
2. objective function
3. choices
4. constraints

LCI Database
(+ User Inventories)



Brightway

Python-based User-defined
Lifecycle Product Optimization

PULPO

Optimization Model

PYOMO

Results

save_results()

pandas

summarize_results()

Conclusions

- Regular maintenance of data and tools enhances the robustness of environmental assessments.
- PSE concepts demonstrated their ability to pioneer large-scale process data creation.
- Accessible data and tools can significantly advance digital sustainability.

Take home message:

Process Systems Engineering can help cover data gaps in LCA and enable the optimization of large-scale systems to guide the future sustainable transition

Acknowledgements

Thank you!

NCCR Catalysis (grant 180544), a National Centre of Competence in Research, Swiss National Science Foundation