Modelling Chemicals in LCA

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GreenDelta GmbH

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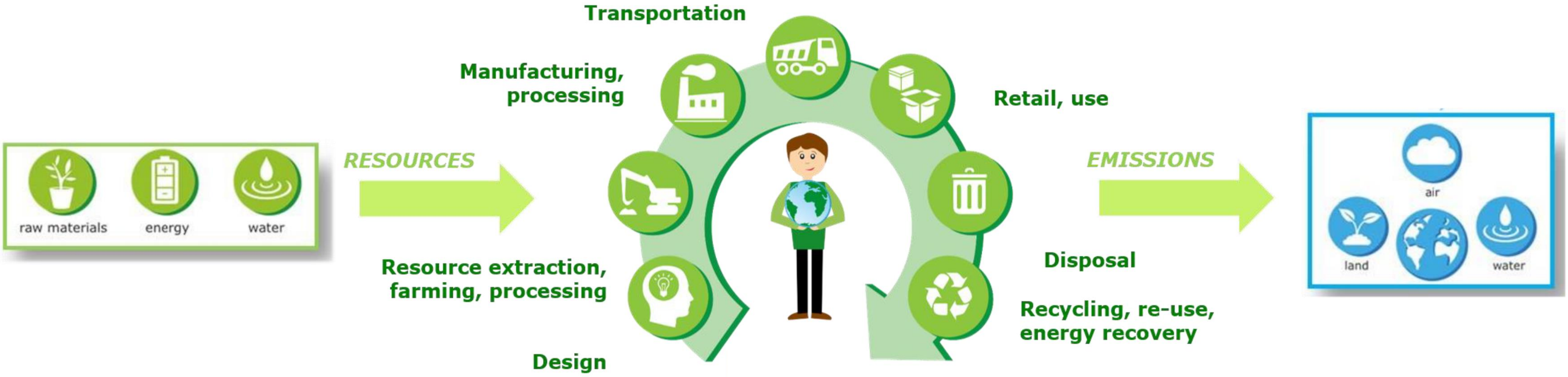
What is LCA?

Definition (ISO 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

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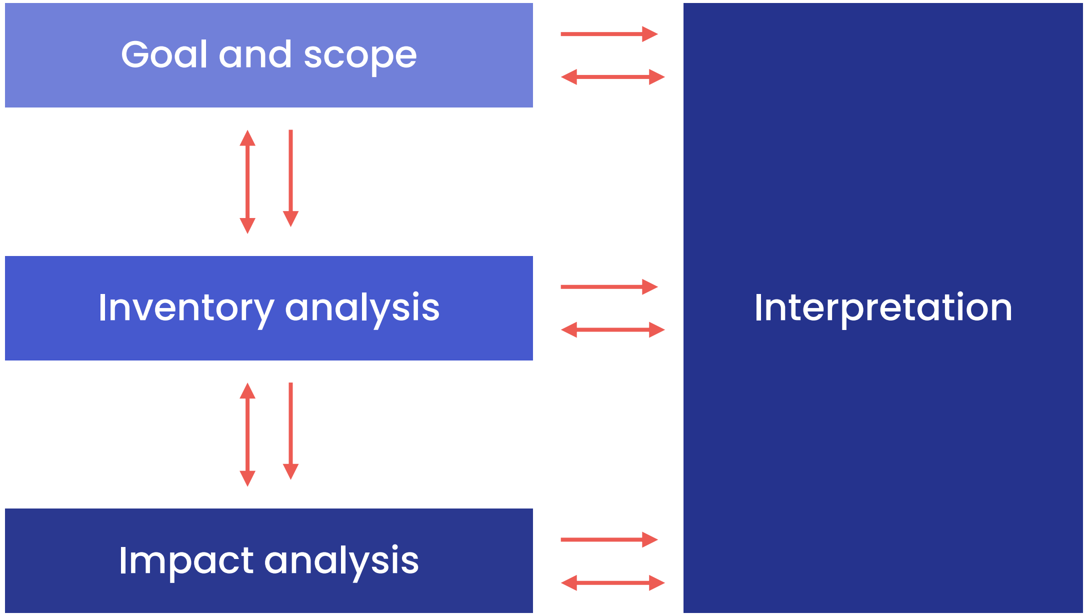
Life Cycle Assessment: Structure

- 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



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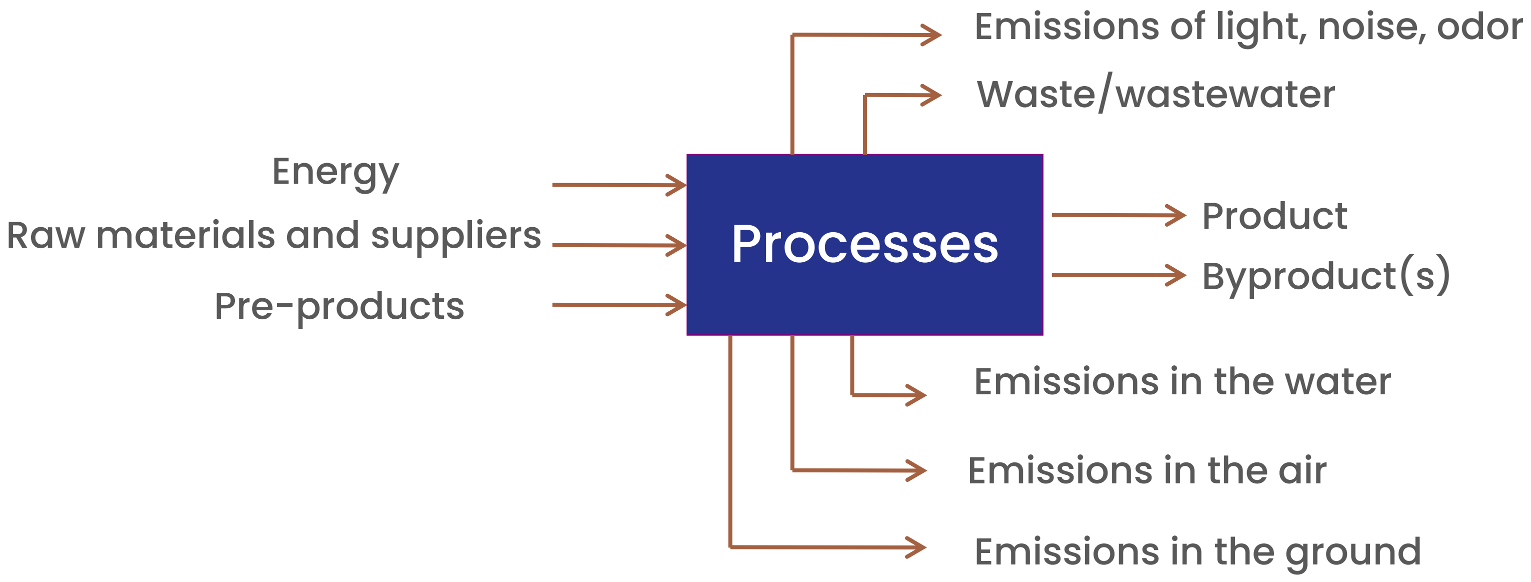
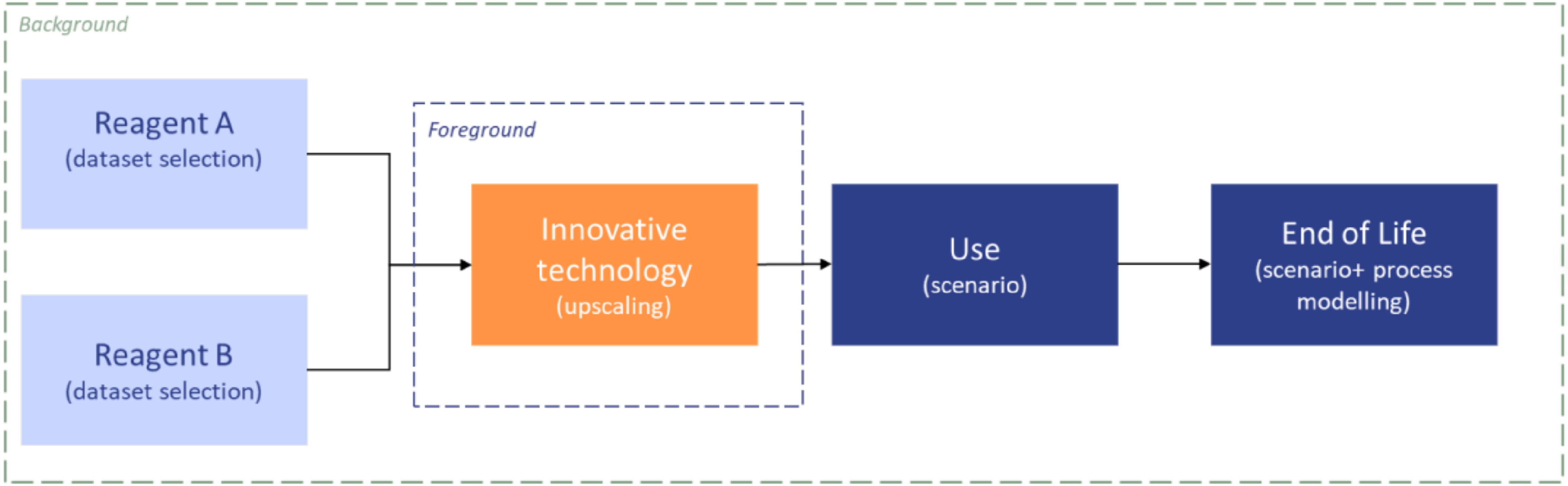
Inputs and outputs of a process to be included in the LCI



Life Cycle Inventory: Data generation and collection



European Commission, Joint Research Centre, Abbate, E., Garmendia Aguirre, I., Bracalente, G., Mancini, L., Tosches, D., Rasmussen, K., Bennett, M.J., Rauscher, H. and Sala, S., Safe and Sustainable by Design chemicals and materials - Methodological Guidance, Publications Office of the European Union, Luxembourg, 2024, https://data.europa.eu/doi/10.2760/28450, JRC138035.

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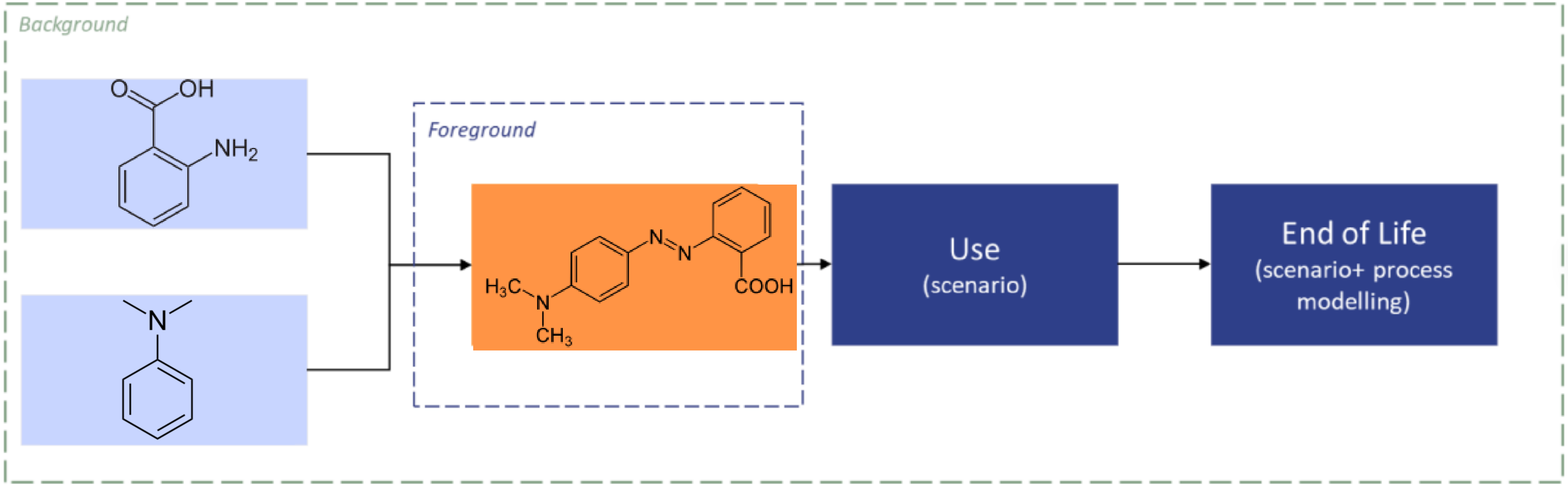
Life Cycle Inventory: Data generation and collection



European Commission, Joint Research Centre, Abbate, E., Garmendia Aguirre, I., Bracalente, G., Mancini, L., Tosches, D., Rasmussen, K., Bennett, M.J., Rauscher, H. and Sala, S., Safe and Sustainable by Design chemicals and materials - Methodological Guidance, Publications Office of the European Union, Luxembourg, 2024, https://data.europa.eu/doi/10.2760/28450, JRC138035.

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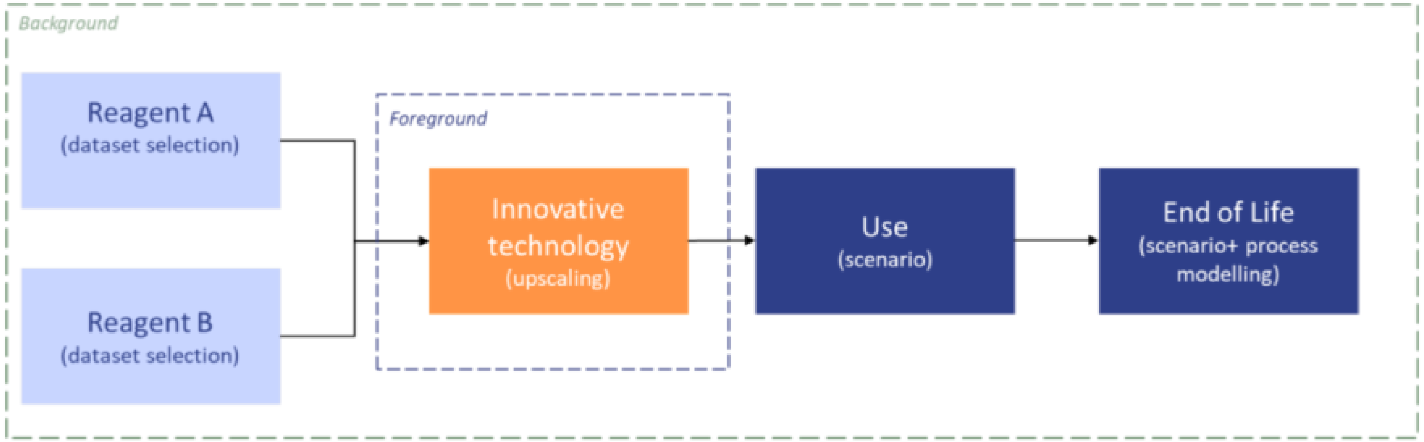

background databases

ecoinvent

carbonminds

EF 3.1 DB

GaBi Database Content

European Commission, Joint Research Centre, Abbate, E., Garmendia Aguirre, I., Bracalente, G., Mancini, L., Tosches, D., Rasmussen, K., Bennett, M.J., Rauscher, H. and Sala, S., Safe and Sustainable by Design chemicals and materials - Methodological Guidance, Publications Office of the European Union, Luxembourg, 2024, https://data.europa.eu/doi/10.2760/28450, JRC138035.

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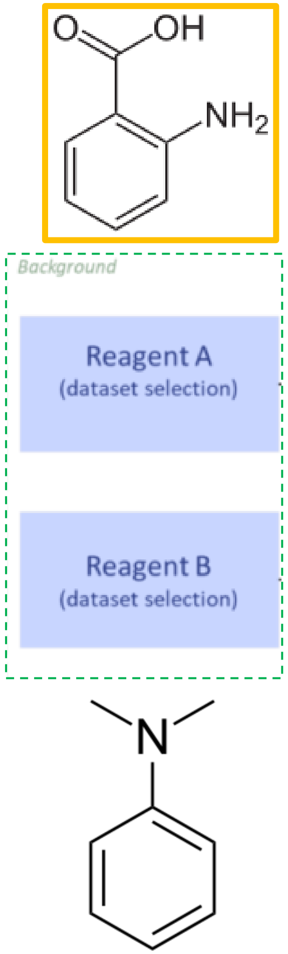
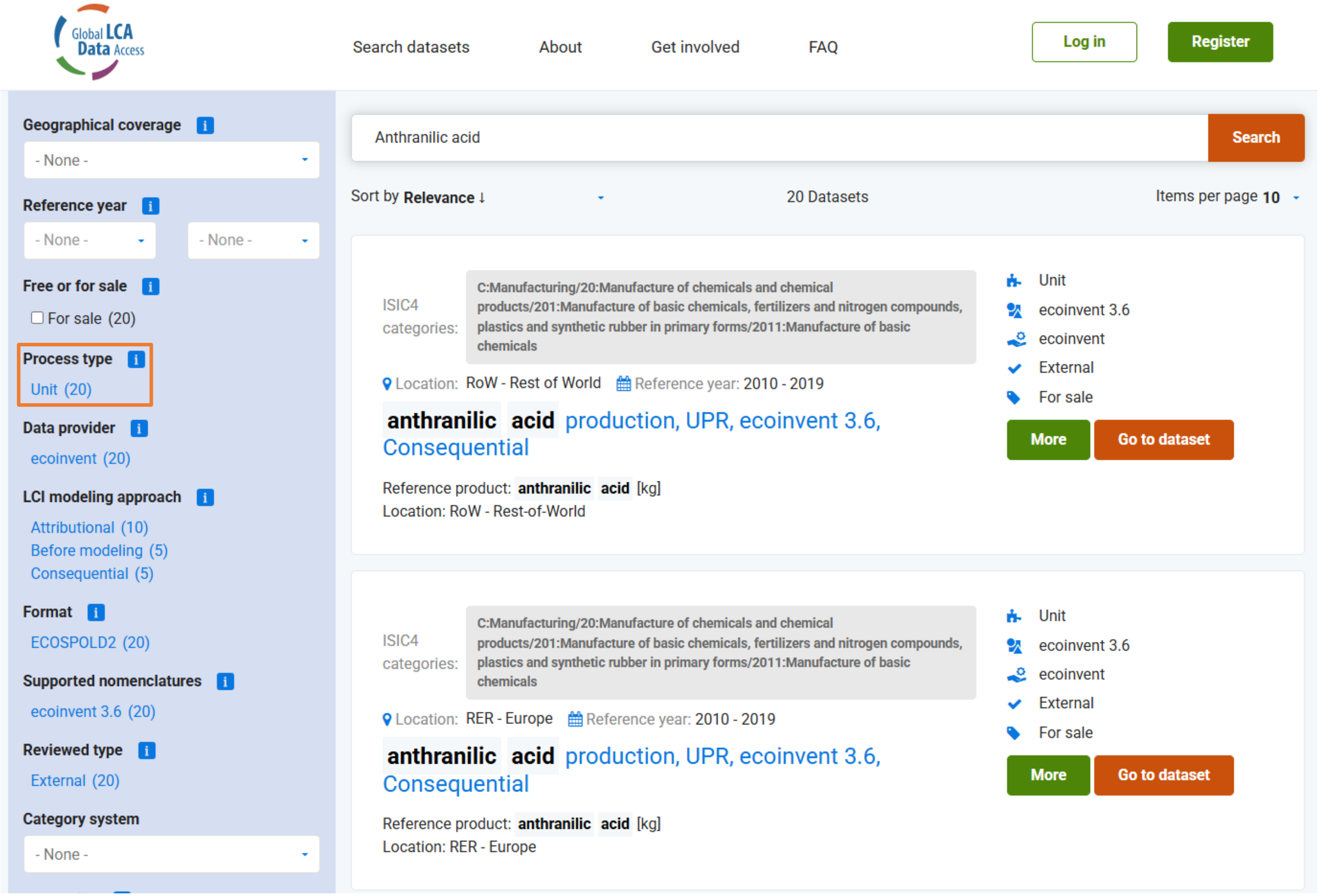
Life Cycle Inventory: Dataset selection





https://www.globallcadataaccess.org/search

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Where to LCI for chemicals?

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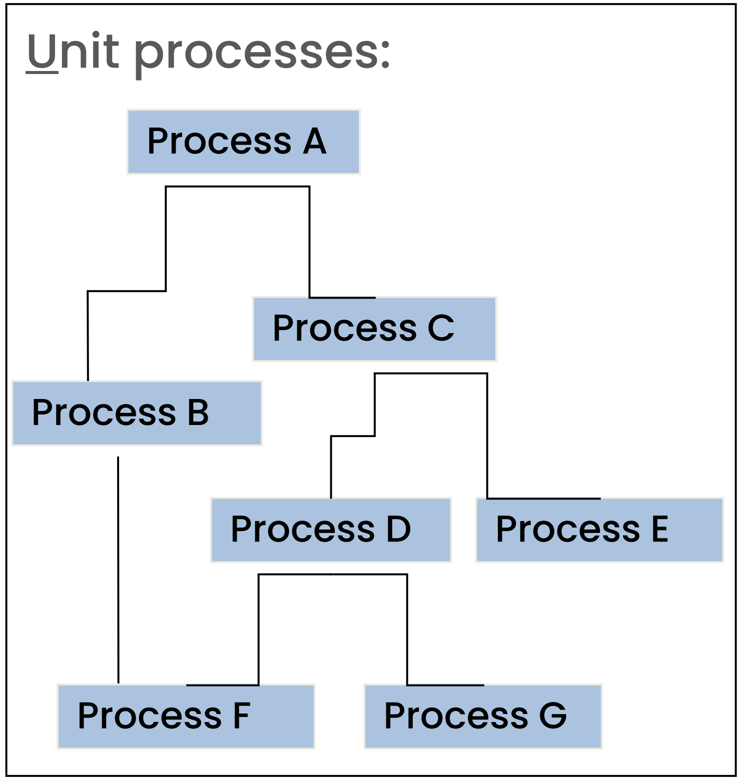
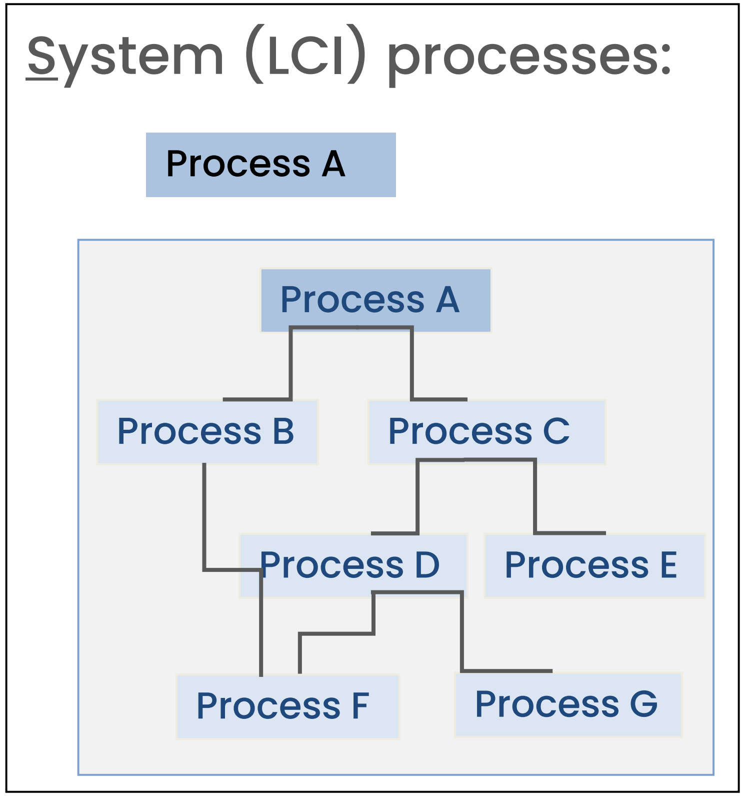
EF 4.0 DB





carbonminds

PLASTICS EUROPE
Enabling a sustainable future

GaBi
Database Content

EF 3.1 DB

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Datasets in LCI databases: Bicycle

Inputs/Outputs: bicycle production | bicycle | Cutoff, U - RER

Inputs

Flow	Category	Amount	Unit	Costs/Re...	Uncertai...	Avoided
Aluminium	Resource/in ground	6.22153	kg		none	
Anhydrite	Resource/in ground	1.31351E...	kg		none	
Antimony	Resource/in ground	2.24515E...	kg		none	
Argon-40	Resource/in air	0.02252	kg		none	
Arsenic	Resource/in ground	7.53473E...	kg		none	
Barium	Resource/in ground	0.06701	kg		none	
Basalt	Resource/in ground	0.00900	kg		none	
Borax	Resource/in ground	1.04062E...	kg		none	
Boron	Resource/in ground	8.36654E...	kg		none	
Bromine	Resource/in water	1.35318E...	kg		none	
Cadmium	Resource/in ground	1.50582E...	kg		none	
Calcite	Resource/in ground	4.12170	kg		none	

Outputs

Flow	Category	Amount	Unit	Costs/Re...	Uncertai...	Avoided
1,2-Dichlorobenze...	Emission to air/high ...	2.98856E...	kg		none	
1,2-Dichlorobenze...	Emission to water/su...	9.07175E...	kg		none	
1,3-Dioxolan-2-one	Emission to water/u...	1.35174E...	kg		none	
1,4-Butanediol	Emission to air/high ...	2.17547E...	kg		none	
1,4-Butanediol	Emission to water/su...	5.00358E...	kg		none	
1-Pentanol	Emission to air/high ...	1.43931E...	kg		none	
1-Pentanol	Emission to water/su...	3.45437E...	kg		none	
1-Pentene	Emission to air/high ...	1.67038E...	kg		none	
1-Pentene	Emission to water/su...	2.61042E...	kg		none	
2,2,4-Trimethyl pe...	Emission to air/unsp...	9.16497E...	kg		none	
2,4-D	Emission to air/low ...	6.56607E...	kg		none	
2,4-D	Emission to soil/agri...	7.32983E...	kg		none	

General information | Inputs/Outputs | Administrative information | Modeling and validation | Parameters | Allocation

Inputs/Outputs: bicycle production | bicycle | Cutoff, U - RER

Inputs

Flow	Category	Amount	Unit
aluminium, wrought alloy	242:Manufacture of ...	7.53250	kg
chromium steel removed by turning, average, co...	259:Manufacture of ...	0.15900	kg
electricity, medium voltage	351:Electric power g...	6.89020	kWh
heat, district or industrial, natural gas	353:Steam and air co...	13.58025	MJ
heat, district or industrial, other than natural gas	353:Steam and air co...	0.19270	MJ
injection moulding	222:Manufacture of ...	1.95750	kg
polyethylene, high density, granulate	201:Manufacture of ...	1.95750	kg
polyurethane, flexible foam	201:Manufacture of ...	0.03000	kg
powder coat, aluminium sheet	259:Manufacture of ...	0.35000	m2
road vehicle factory	410:Construction of ...	9.36930E...	Item(s)
section bar extrusion, aluminium	242:Manufacture of ...	3.76630	kg

Outputs

Flow	Category	Amount	Unit
bicycle	**309:Manufacture o...**	**1.00000**	**Item...**
municipal solid waste	382:Waste treatment...	4.50000	kg
used bicycle	383:Materials recove...	1.00000	Item(s)
wastewater, average	370:Sewerage/3700:S...	0.00073	m3
wastewater, average	370:Sewerage/3700:S...	1.82394E...	m3
Water	Emission to air/unsp...	0.00011	m3

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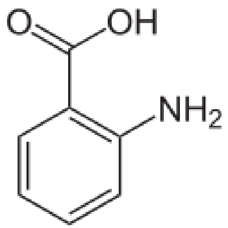
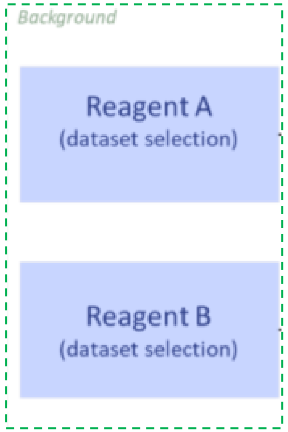
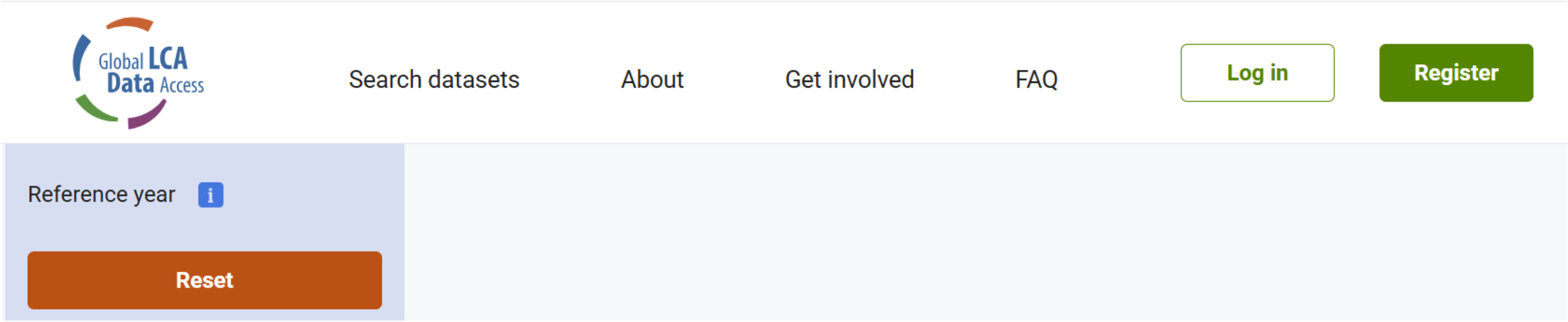
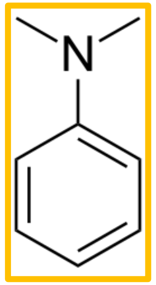
Life Cycle Inventory: Dataset selection









What to do if there is no data available?

https://www.globallcadataaccess.org/search

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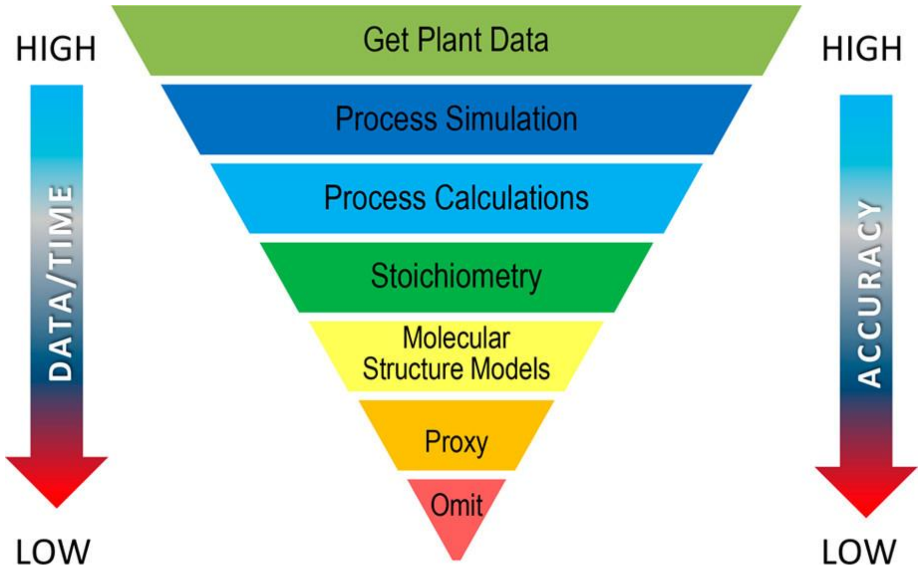
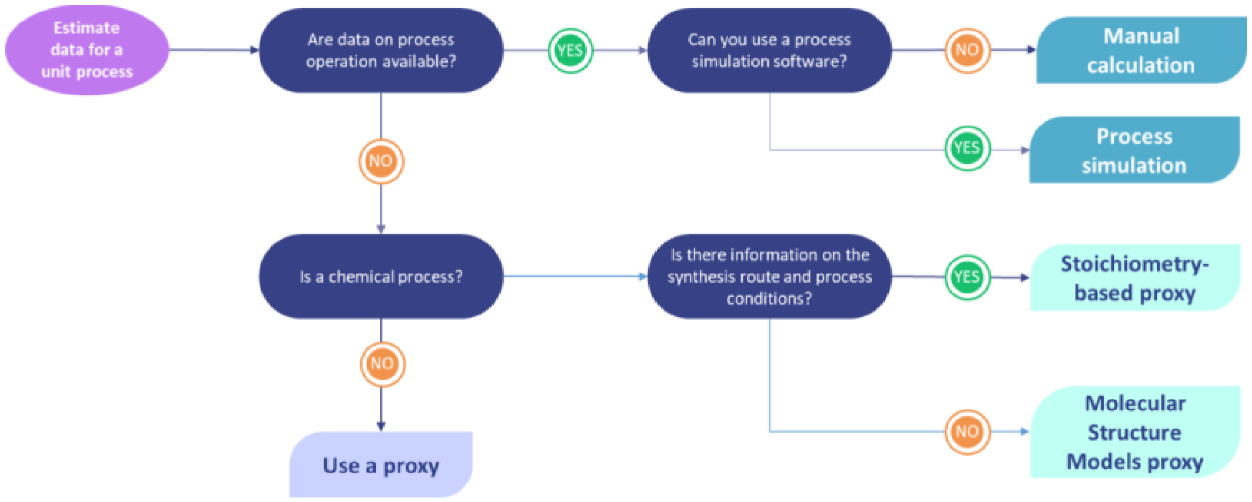
Life Cycle Inventory – Data needed





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

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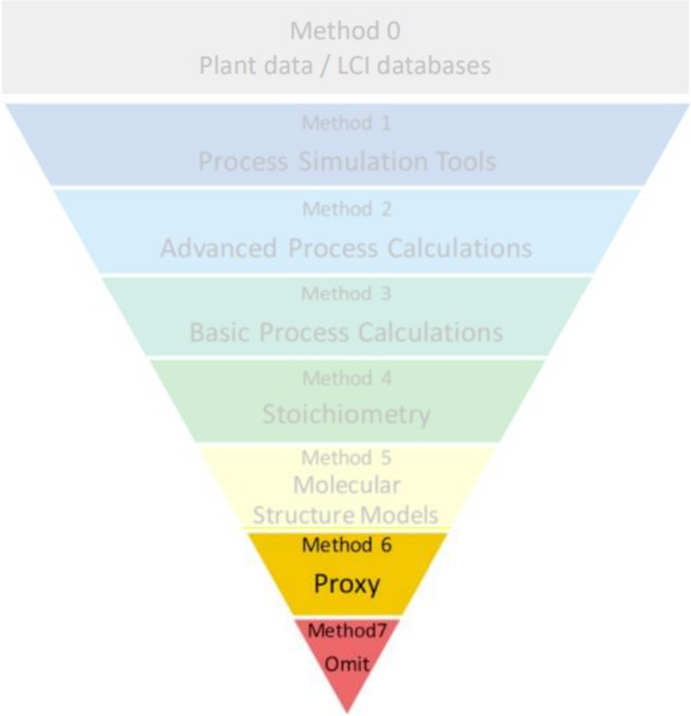
How to fill data gaps for chemical LCIs?

Method 6 and 7:



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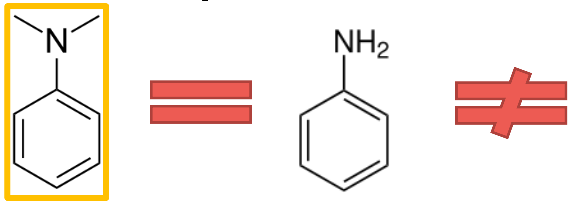
Proxy:

- Relies on existing LCI data of similar (proxy) chemicals
- Used when no synthesis or stoichiometric data is available

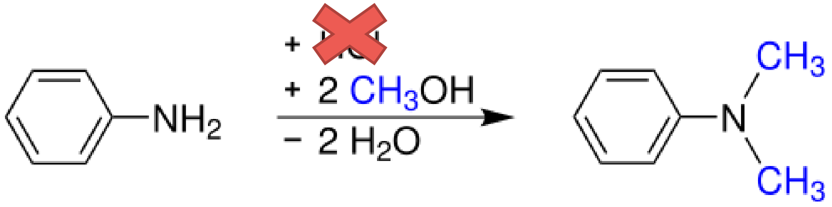


market for chemical, organic | chemical, organic | Cutoff, U - GLO
C:Manufacturing/20:Manufacture of chemicals and chemical products/2
#Chemicals

market for chemical, inorganic | chemical, inorganic | Cutoff, U - GLO
C:Manufacturing/20:Manufacture of chemicals and chemical products/2
#Chemicals

Omitting:

- Least preferred, yet common when data is missing
- Impacts fall below defined cut-off criteria (e.g., <5% of mass)
  e.g. catalyst, additives



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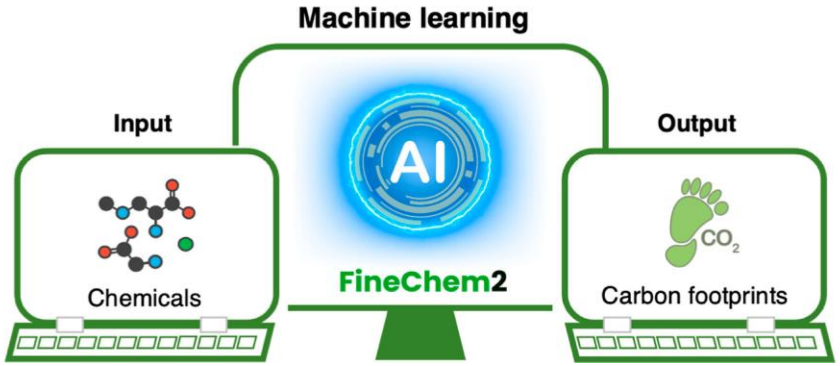
How to fill data gaps for chemical LCIs?

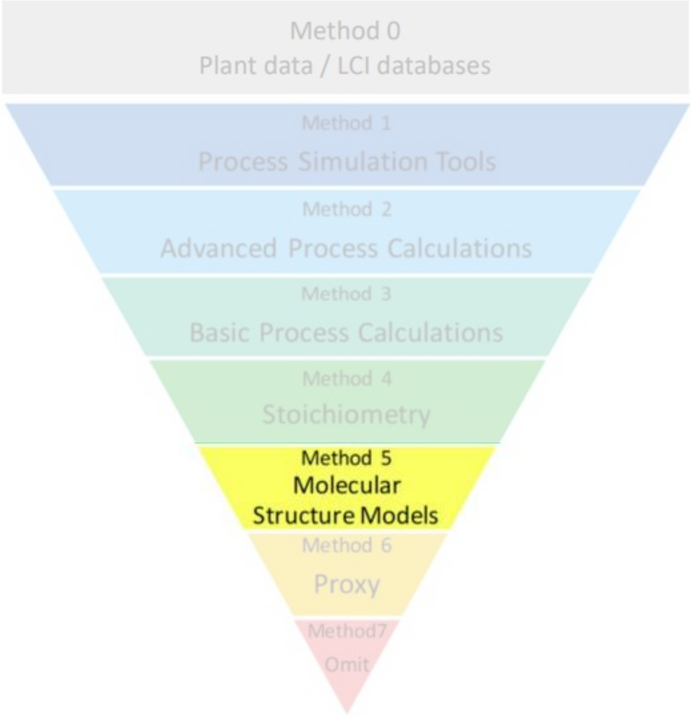
Method 5:
Molecular Structure Models (QSARs)



$$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{n}(Y_i - f(x_i))^2}$$

$$\text{mean PE} = \frac{100\%}{n}\sum_{i=1}^{n}\frac{|Y_i - f(x_i)|}{Y_i}$$

$$\text{median PE} = \text{median}\left(\frac{|Y_i - f(x_i)|}{Y_i}\right)$$



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

G. Wernet et. al., *Green Chemistry* **2009**, 11 (1826), D. Zhang et. al., *ACS Sustainable Chem. Eng.* **2024**, 12 (2007).

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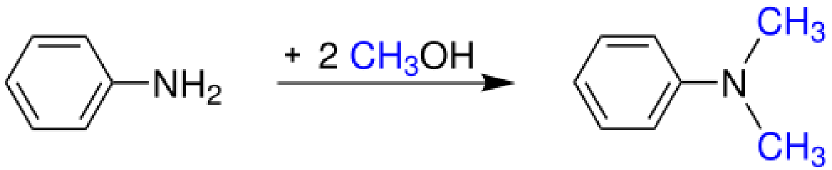
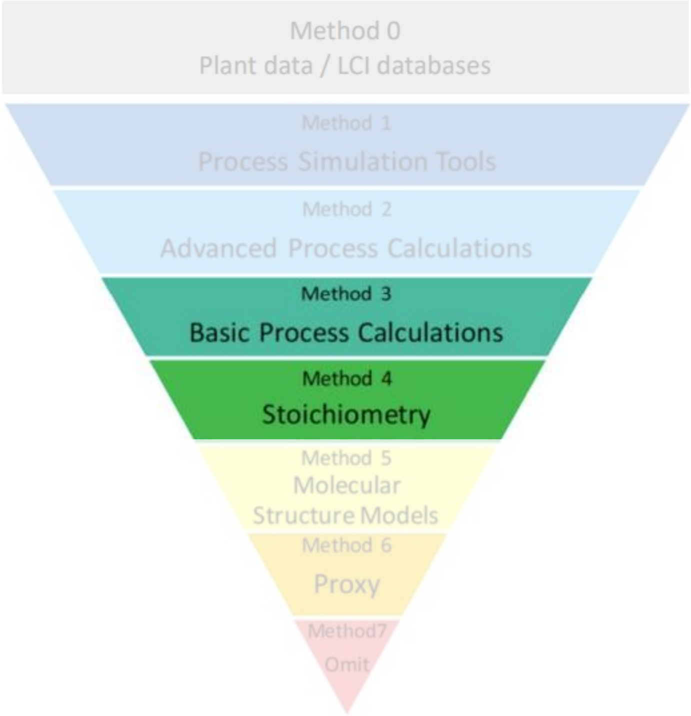
How to fill data gaps for chemical LCIs?

Method 4:

Basic and Stochiometric Calculations



- 1. eq. Aniline + 2 eq. MeOH → Dimethylaniline
- Consult literature for routes (Ullmann, patents, Best Available Technqiue)
- Add „Gendorf Approach"
  - 2.2 MJ , 0.4 kWh , 95% yield per kg produced chemical
  - Access starting material concerted to CO2
  - Water consumption and waste generic



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

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

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How to fill data gaps for chemical LCIs?

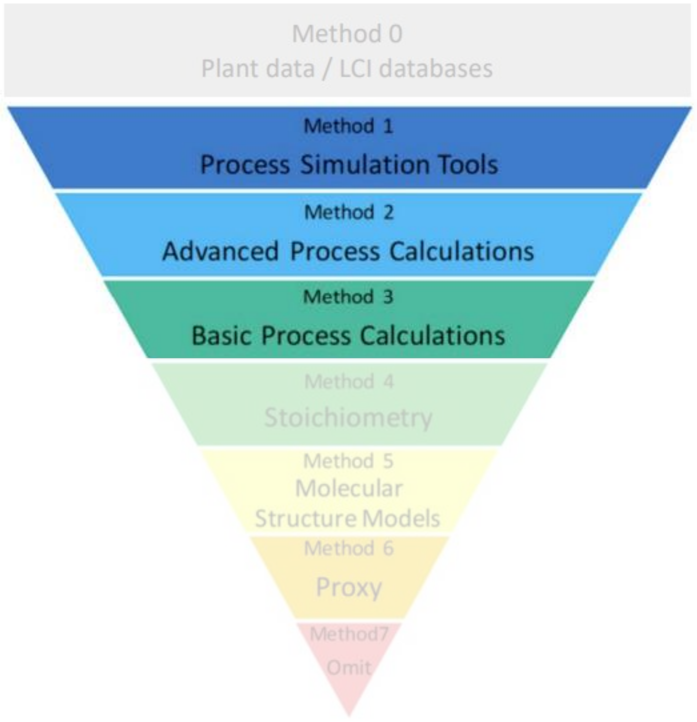
Method 1 and 2, 3:

Method 1: Process Simulation Tools

- Uses software (e.g., Aspen Plus, DWSIM) to model reaction
- Ideal for non-commercial or novel chemicals

Method 2 and 3: Process Calculations

- Basic: Uses mass & energy balance equations and empirical rules
- Basic: Assumes static operating conditions
- Adv.: Adds detail: equipment efficiency, heat loss, reactor design
- Adv.: More precise estimates of energy and emissions



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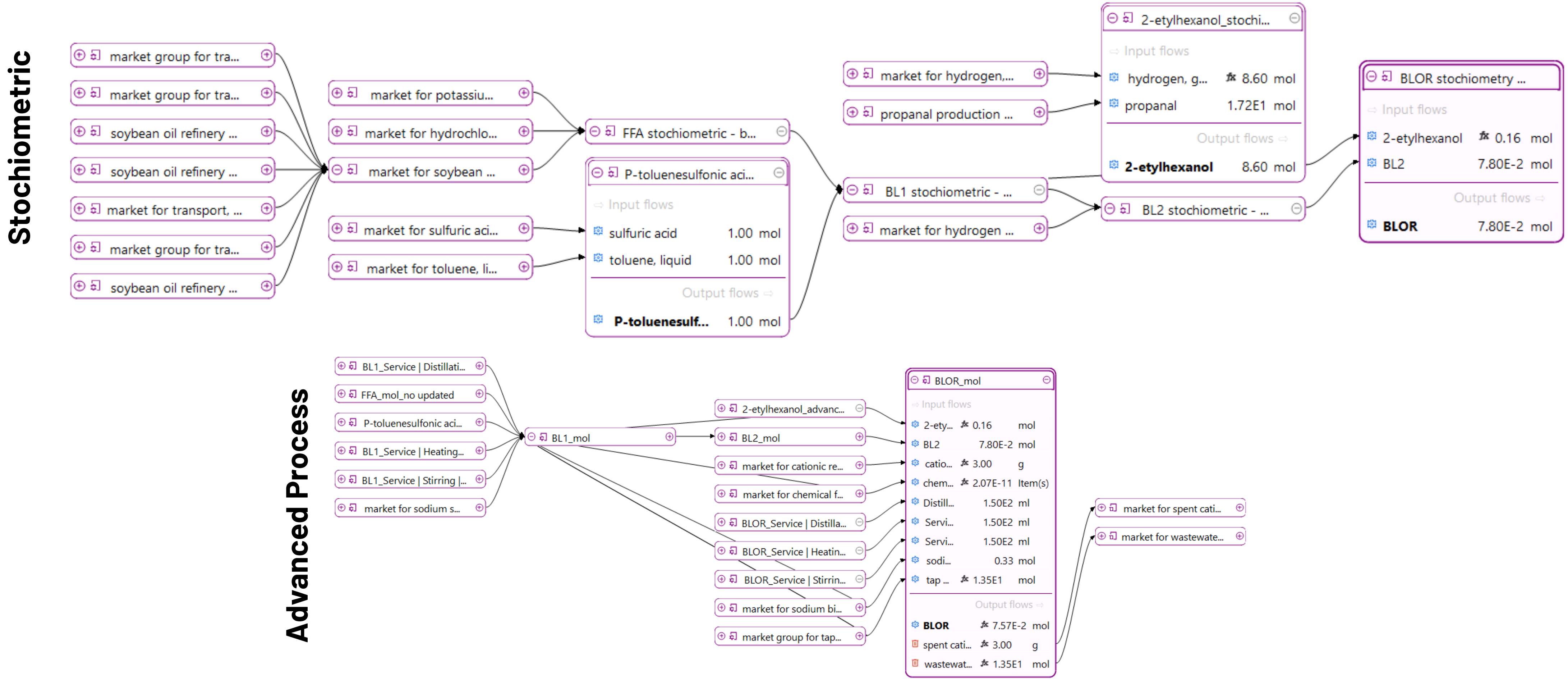
Issues than can arrives

Method 2, 3 and 4 in comparison



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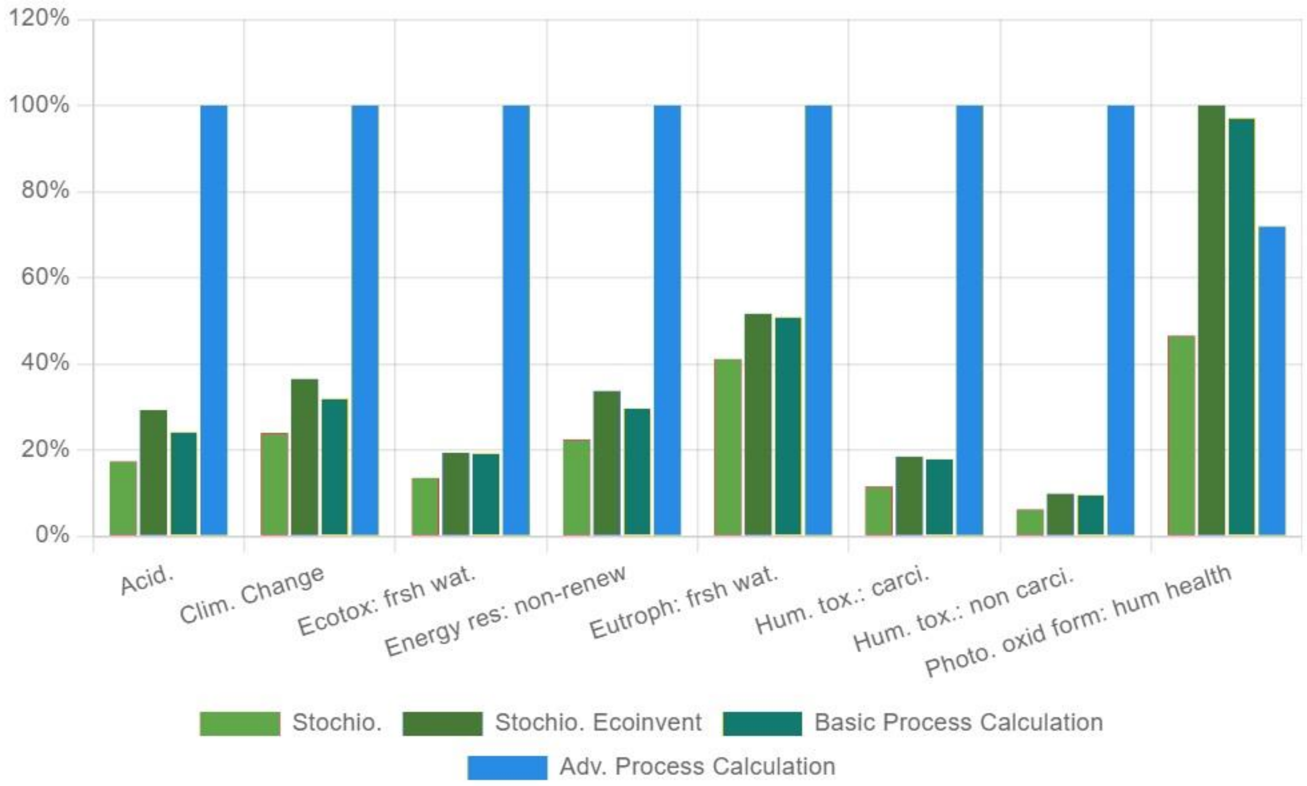
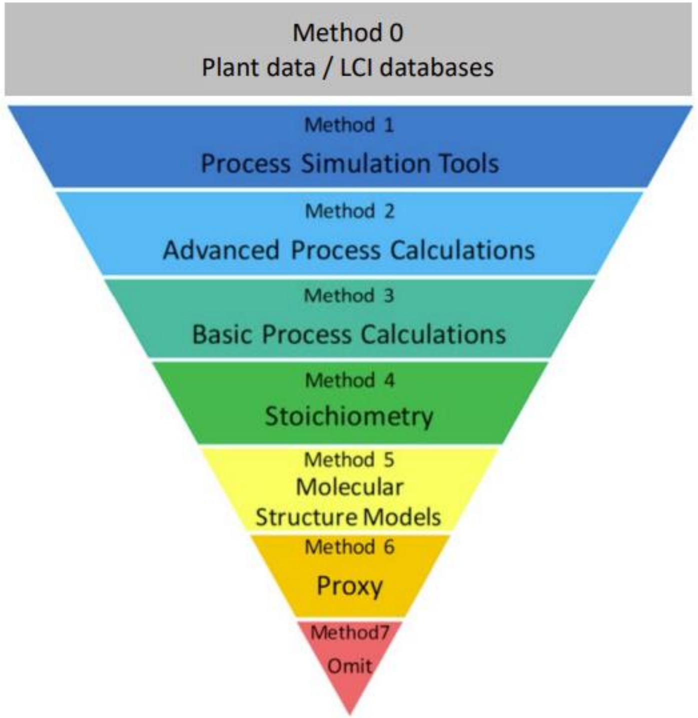
Method 2, 3 and 4 in comparison





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How to fill data gaps for chemical LCIs?

Method 0:
Plant / LCI databases

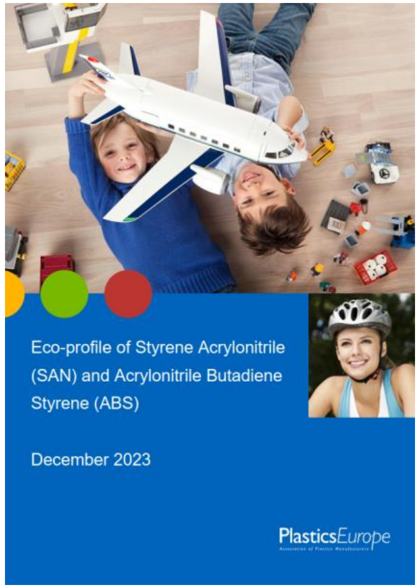
ecoinvent

carbonminds

EF 3.1 DB

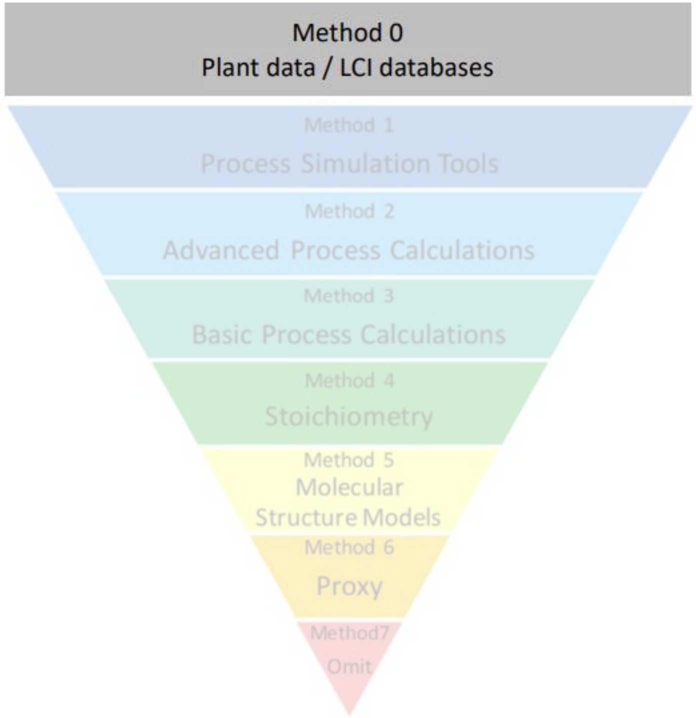
GaBi Database Content

LCI databases



Plant/lit. data

https://plasticseurope.org/sustainability/circularity/life-cycle-thinking/eco-profiles-set/



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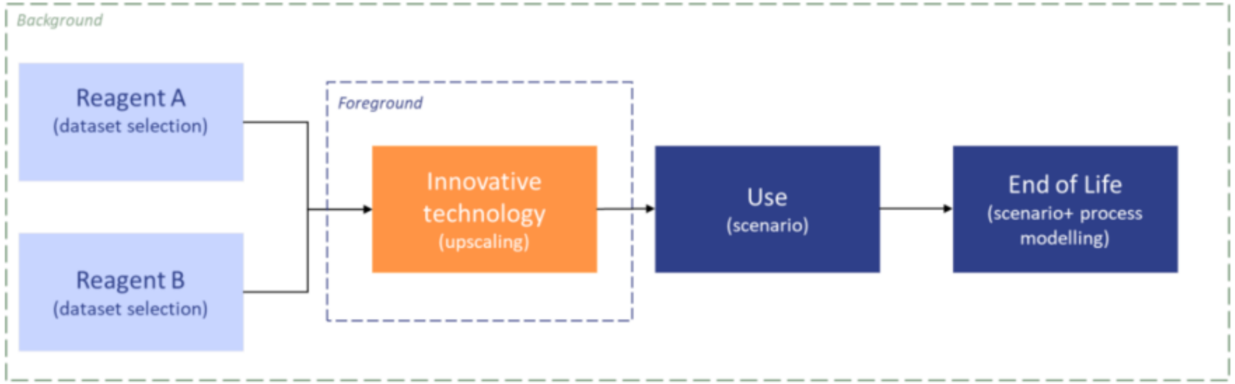
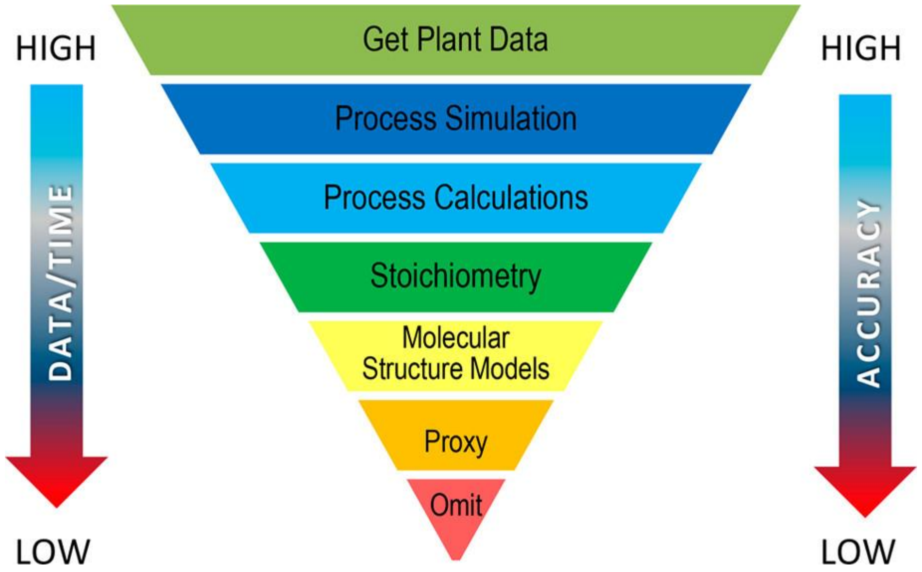
Conclusion





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

- Background vs. Foreground
- Where to find data (System vs. Unit Processes)
- Depending on information level we can fill data gaps with different methods

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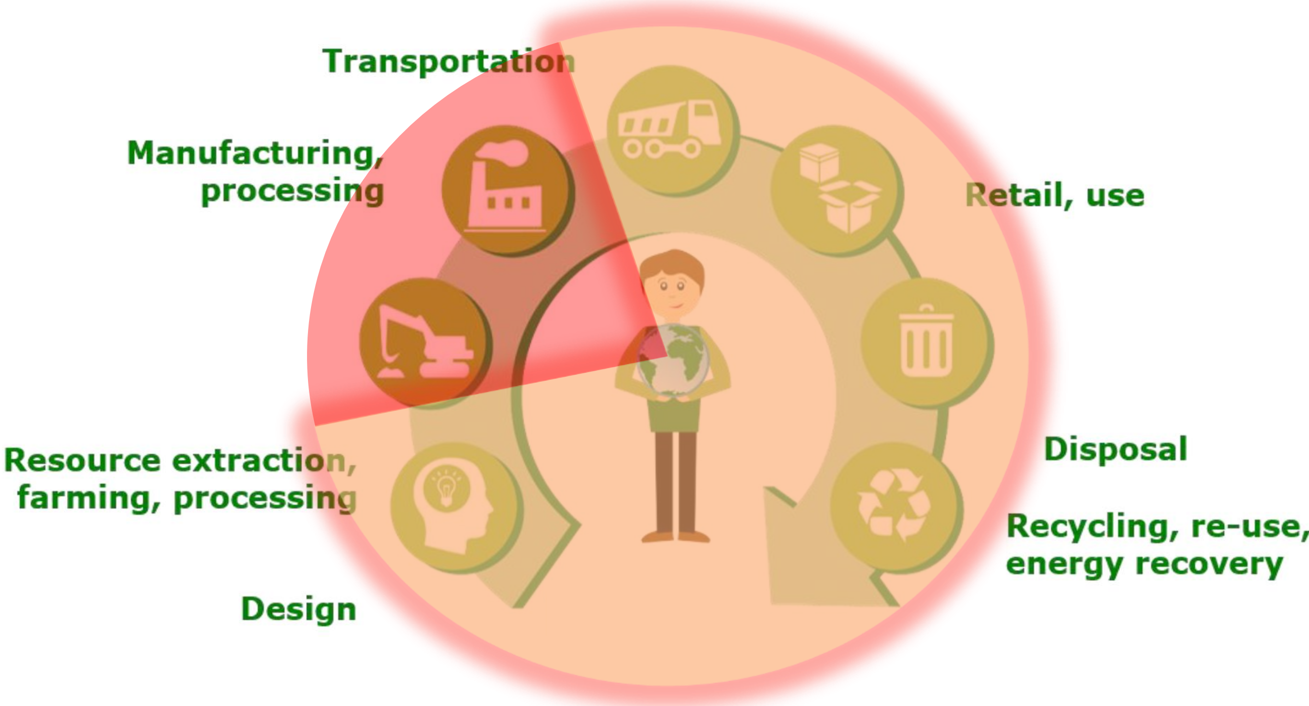
Final Remarks

- We focused now on production
- However, use phase and EoL are also relevant but more complex to describe
- The full life cycle has to be tracked until the material is emitted to environment
  - Recyclability
  - Fate of materials
  - Biodegradability and persistency



Thanks

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