



SITOLUB

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

Assessing Modelling Approaches in Chemical LCA Databases to Quantify Cumulative Uncertainty

23/04/2026

openLCA.conf 2026

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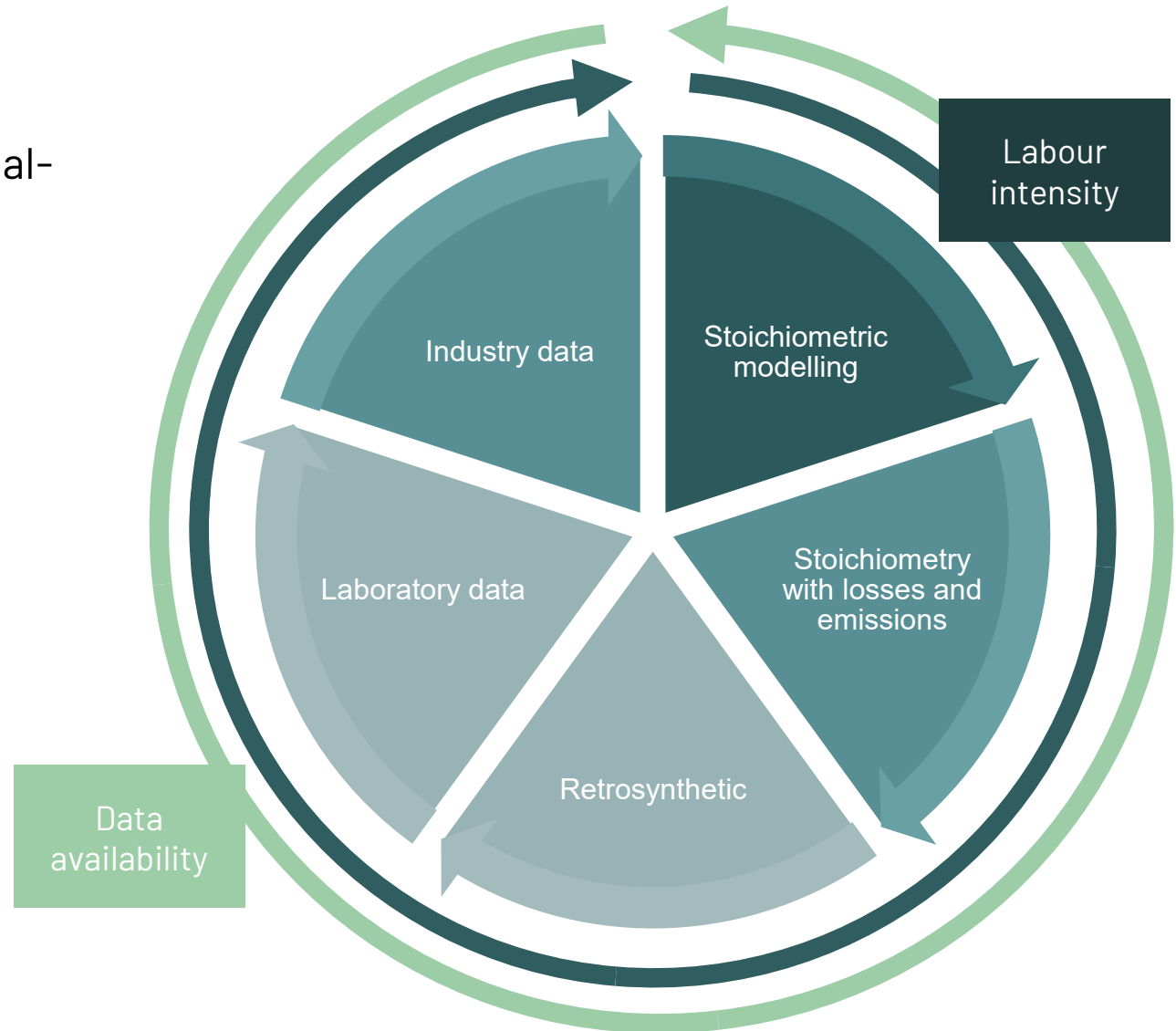
GreenDelta

Introduction

- The chemical industry is responsible for ~10% of annual global CO2 emissions
- Frameworks to deliver lower-risk higher-sustainability data for are being elaborated upon
 - Safe and Sustainable by Design (SSbD)
- LCA background databases are ill-equipped to handle complex and diverse chemical supply chains
 - **>100000 compounds** in commerce, **only a few hundred modelled**
- **Machine learning** approaches to **rapidly quantify environmental risks** of chemicals are
 - Background data is required for their application
 - Therefore, we had a **critical look at chemical modelling** in widespread environmental databases

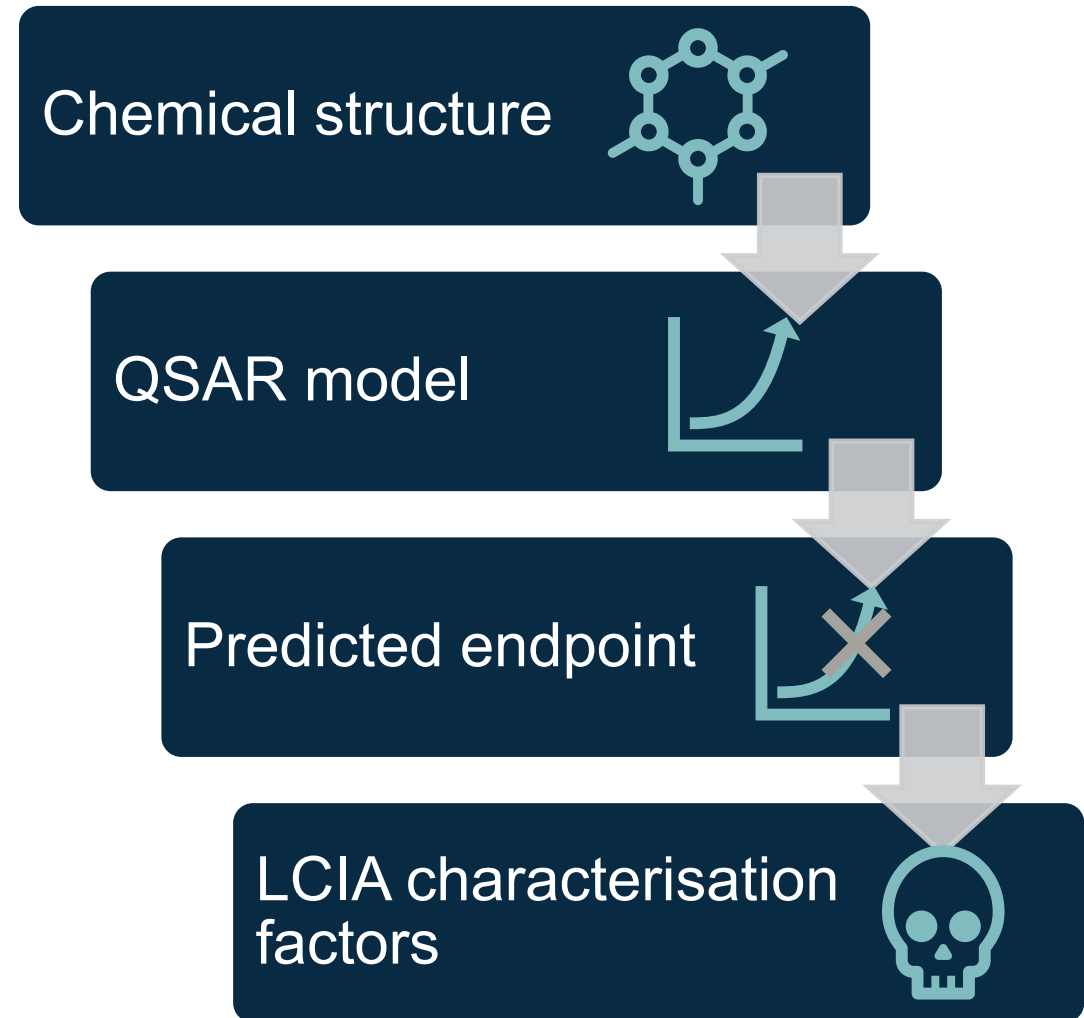
Chemical production modelling approaches

- Empirical and theoretical approaches
- Extension of pure stoichiometry to reflect real-world conditions via assumptions and estimations
- Approach often applied in state-of-the-art chemical production modelling
- Trade-offs between model granularity, representativeness, data availability and requirements across approaches
- Feasibility to integrate into automated approaches varies



Machine learning to estimate impacts

- Quantitative structure–activity relationship (QSAR) predicts chemical properties and toxicity
- In LCIA, QSAR helps fill data gaps for ecotoxicity, human toxicity, persistence, and bioaccumulation
- Predictions based on similar chemistry can be used to estimate characterization factors (CFs)
- QSAR is especially useful for screening large chemical inventories and prioritizing substances for further assessment



Generic modelling of chemicals in ecoinvent



Input	Amount for reference year 2024
Natural gas [GJ]	4,057,000
Electricity [GJ]	2,503,300
Water, tap [t]	51,157
Water, well [t]	16,428,000
Water, river [t]	18,586,000
Nitrogen [Nm ³]	34,878,000
Compressed air [Nm ³]	792,800,000
Oxygen [Nm ³]	106,510,000
Land use, total [m ²]	1,998,100
Produced chemicals [t]	1,366,400



Generic modelling of chemicals in ecoinvent

Inputs/Outputs - 2,4-dichlorophenol production | 2,4-dichlorophenol | Cutoff, U - RER

Flow	Amount	Unit	Uncerta...	Data quali...	Description
chemical fa...	4.00000E-10	lte...	lognor...	(2; 4; 5; 4; 4)	Calculated based on literature data published by the industry. For this acti
chlorine, li...	0.90968	kg	lognor...	(4; 5; 5; 1; 1)	As there was no data available for the production of 2,4-dichlorophenol, tl
electricity, ...	0.39906	kWh	lognor...	(2; 4; 5; 4; 4)	Calculated based on literature data published by the GENDORF Chemical I
heat, distric...	1.88647	MJ	lognor...	(2; 4; 5; 4; 4)	Calculated based on literature data published by the GENDORF Chemical I
heat, from ...	0.20781	MJ	lognor...	(2; 4; 5; 4; 4)	Calculated based on literature data published by the GENDORF Chemical I
phenol	0.61079	kg	lognor...	(4; 5; 5; 1; 1)	As there was no data available for the production of 2,4-dichlorophenol, tl

Reliability	Completeness	Temporal correlation	Geographical correlation	Further technological correlation
2 (sometimes 4)	3-5 (usually 4)	At time of creation	1-5 (commonly 4 or 5)	2-5 (usually 4)

Not a viable filter because of variations due to allocated multi-output processes

Chosen method

Final method applied to ecoinvent

estimated with data from Kim 2003, who gives data for th

0.39906	kWh	L...	market gro...	(2; 4; 3; 5; 4)	Calculated based on literature data published by the GENDORF
1.88647	MJ	L...	market gro...	(2; 4; 3; 5; 4)	Calculated based on literature data published by the GENDORF
0.17666	MJ	L...	market for ...	(2; 4; 3; 5; 4)	Calculated based on literature data published by the GENDORF
0.03115	MJ	L...	market for ...	(2; 4; 3; 5; 4)	Calculated based on literature data published by the GENDORF
0.01471	m3	L...		(2; 4; 3; 5; 4)	Calculated based on literature data published by the GENDORF
0.00097	m3	L...		(2; 4; 3; 5; 4)	Calculated based on literature data published by the GENDORF
0.00082	m3	L...		(2; 4; 3; 5; 4)	Calculated based on literature data published by the GENDORF

According to Chauvel and Lefebvre (1989),
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0.39906	kWh	L...	market gro...	(2; 4; 3; 5; 4)	Calculated based on literature data published by the GENDORF
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0.00082	m3	L...		(2; 4; 3; 5; 4)	Calculated based on literature data published by the GENDORF

Highly generic:
 >3 Gendorf flows

Generic data:
 filtered by
 identifiers/description

Partially generic:
 remaining fraction

All processes contained in category
 201: manufacture of basic chemicals,
 fertilizers and nitrogen compounds, plastics

Remaining processes

Heat as reference product:
 filtered by flow

Market proces
 filtered by na

Cooling
 pH modifiers
 Catalyst (Nickel class 1, ...)
 Water

Water, cooling, unspecified n...	0.01471	m3	(2; 4; 3; 5; 4)	Calculated based on literature data published by the GENDORF
Water, river	0.00097	m3	(2; 4; 3; 5; 4)	Calculated based on literature data published by the GENDORF
Water, well, in ground	0.00082	m3	(2; 4; 3; 5; 4)	Calculated based on literature data published by the GENDORF

PlasticsEurope/ECVM2023

PlasticsEurope2016

PlasticsEurope2016

PlasticsEurope2016

PlasticsEurope2017

IEAGHG2017

IFEU/PlasticsEurope2021

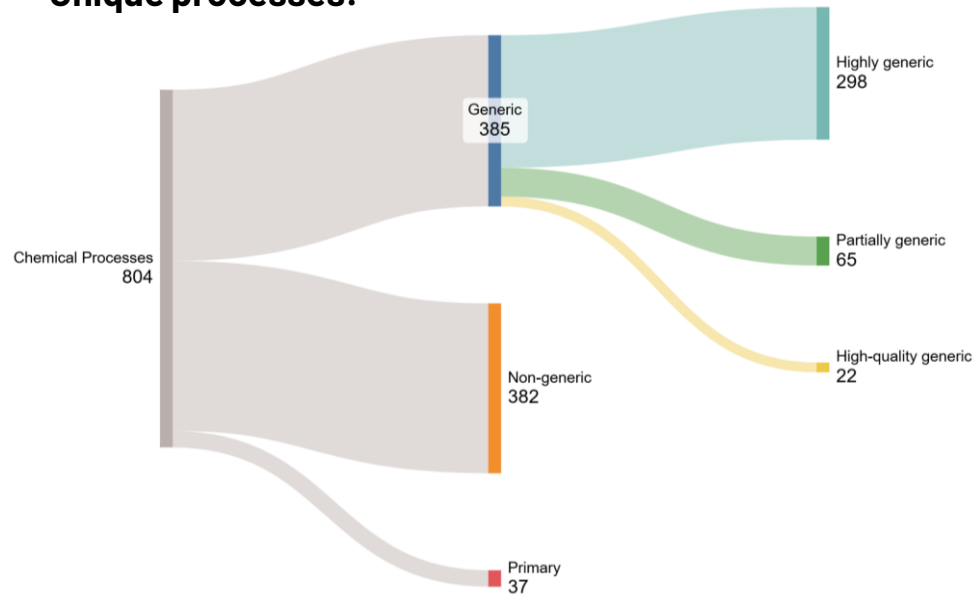
IFEU/PlasticsEurope2021

International Aluminium Insitute2015

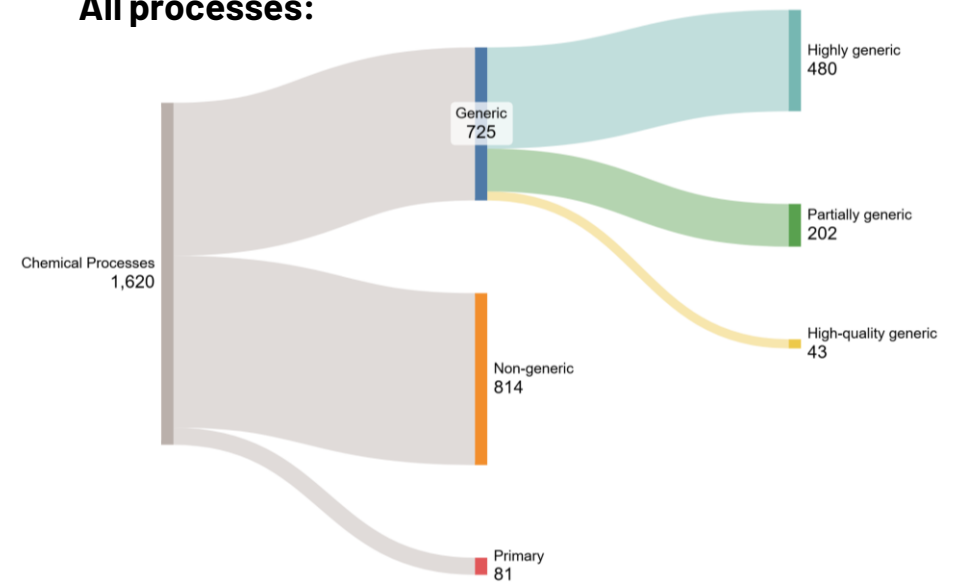
steam and air condition...	0.13400	kWh	lognormal: gmean...	market group f...	(1; 2; 3; 1; 1)	Value based on a company survey by PlasticsEurope (three companies and four production
/19:Manufacture of cok...	0.28100	kg	lognormal: gmean...	market for ethy...	(1; 2; 3; 1; 1)	Value based on a company survey by PlasticsEurope (three companies and four production
steam and air condition...	1.50000	MJ	lognormal: gmean...	market group f...	(1; 2; 3; 1; 1)	Value based on a company survey by PlasticsEurope (three companies and four production
steam and air condition...	1.70000	MJ	lognormal: gmean...	market group f...	(1; 2; 3; 1; 1)	Value based on a company survey by PlasticsEurope (three companies and four production
/20:Manufacture of che...	6.80000	MJ	lognormal: gmean...	market for heat...	(1; 2; 3; 1; 1)	Value based on a company survey by PlasticsEurope (three companies and four production

Results of the classification approach

Unique processes:



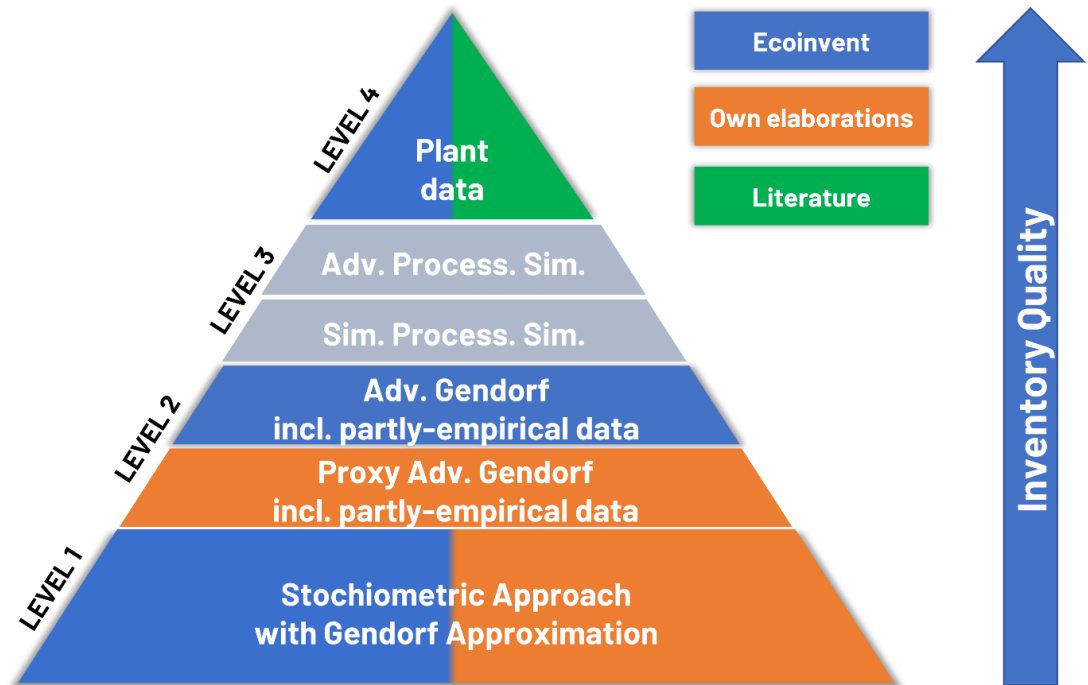
All processes:



	RoW	RER	GLO	Other	RoW	RER	GLO	Other
Non-generic	326	264	39	266	57%	53%	23%	70%
HQ generic	61	53	39	19	11%	11%	23%	5%
Partially generic	72	83	16	85	13%	17%	9%	22%
Highly generic	112	99	76	10	20%	20%	45%	3%

Outlook: classification and uncertainty approach

- We recommend **using the transparency provided by the ecoinvent database** and to **develop a data quality workflow** to be implemented in machine learning methods. openLCA allows to compute data quality uncertainties. **Uncertainty should be considered in ML approaches.**
- **In general, generic stoichiometric approaches are not to be avoided;** hotspots often lie deeper in supply chains at the stage of crude material extraction and processing.



Thank you for your attention

Max F. Bringmann

GreenDelta GmbH