sustainability

Supplementary Information

Automation of Life Cycle Assessment—A Critical Review

Bibliometric Analysis

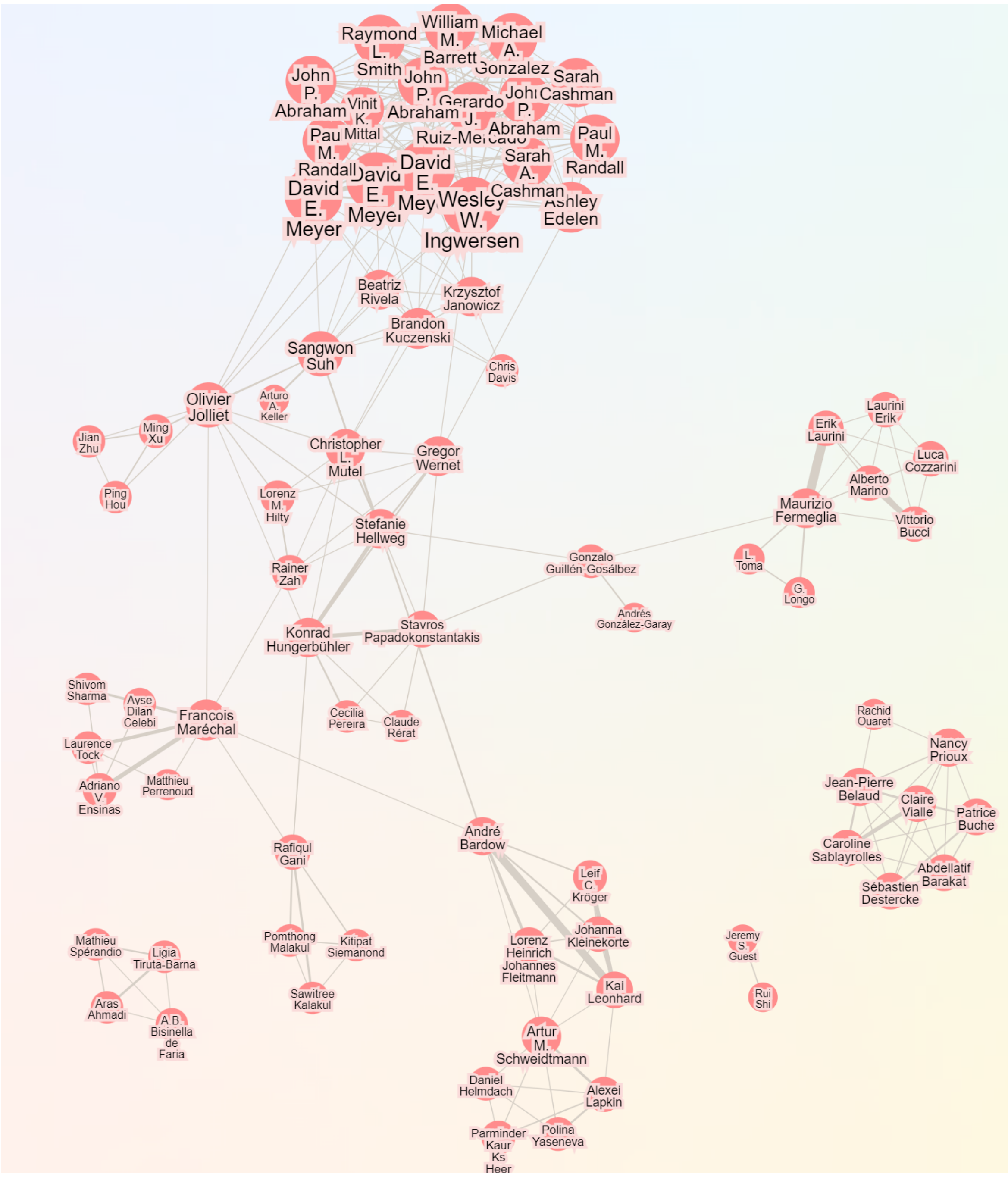

Figure S1. Connection between authors in the analysed papers summarized in **Error! Reference source not found.**. Only the analysed papers, no further research, was used to build this figure [1].

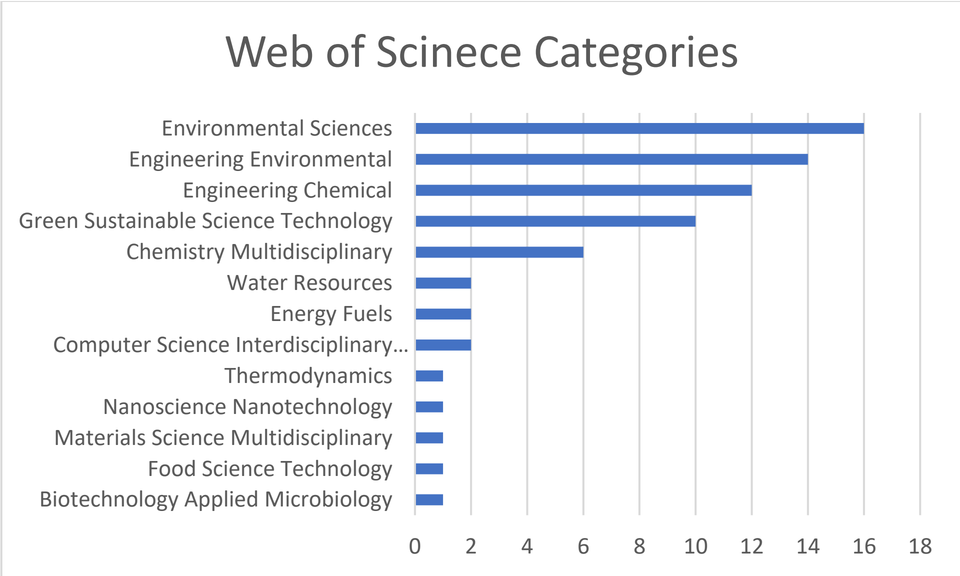

Figure S2. Categories of the analysed papers (n=30) by Web of Science.

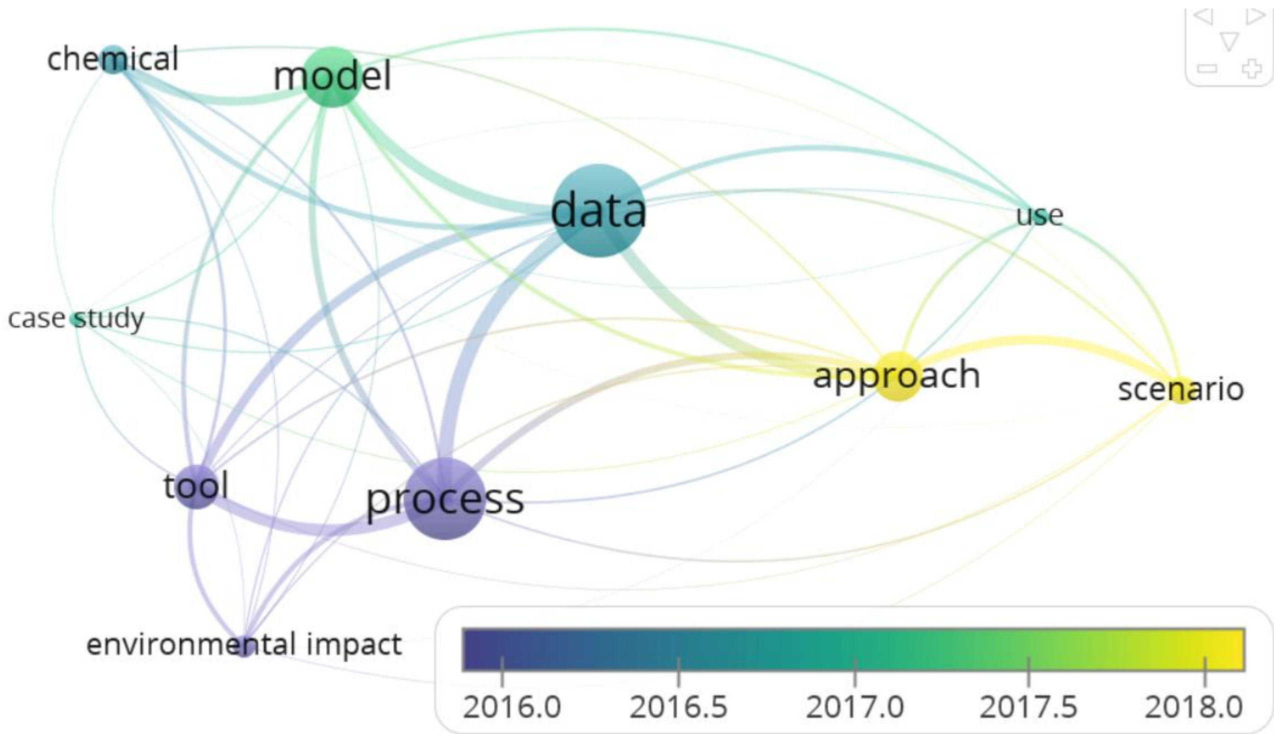

Figure S3. Key word analysis of 30 peer-reviewed publications used for the bibliometric and empirical evaluation; Software: VOSviewer version 1.6.18; Settings: Extraction from Title and Abstract; Minimum number of occurrences of a term- 10; Selection rate = Relevance > 0.5 (not selected terms with this condition were: lca, life cycle assessment, framework and study); Size- Weighted after Occurrence; Scores- Average Publication year [2].

Empirical Analysis

Table S1. Web of Science Analysis by Country/Region (Analysed articles see table S3).

Countries/ Regions	Record Count	% of 31
USA	11	35.484
SWITZERLAND	9	29.032
FRANCE	6	19.355

GERMANY	4	12.903
ITALY	2	6.452
NETHERLANDS	2	6.452
DENMARK	1	3.226
ENGLAND	1	3.226
LUXEMBOURG	1	3.226
SPAIN	1	3.226
SWEDEN	1	3.226
BRAZIL	1	3.226
THAILAND	1	3.226
ECUADOR	1	3.226
MEXICO	1	3.226
SINGAPORE	1	3.226
COTE IVOIRE	1	3.226

Table S2. Web of Science Analysis by Authors of the reviewed publications (source in table S3).

Authors	Record Count	% of 31
Belaud JP	4	12.903
Hungerbuhler K	4	12.903
Ingwersen WW	4	12.903
Meyer DE	4	12.903
Papadokonstantakis S	4	12.903
Barrett WM	3	9.677
Gonzalez MA	3	9.677
Sablayrolles C	3	9.677
Smith RL	3	9.677
Wernet G	3	9.677
Abraham JP	2	6.452
Bardow A	2	6.452
Fermeglia M	2	6.452
Hellweg S	2	6.452
Hou P	2	6.452
Kahn E	2	6.452
Kleinekorte J	2	6.452
Kuczenski B	2	6.452
Leonhard K	2	6.452
Marechal F	2	6.452
Mittal VK	2	6.452
Montrejaud-vignoles M	2	6.452
Pereira C	2	6.452
Vialle C	2	6.452
Xu M	2	6.452
Ahmadi A	1	3.226
Arbuckle P	1	3.226
Azzaro-pantel C	1	3.226
Bailin SC	1	3.226
Barakat A	1	3.226
Baudin I	1	3.226
Benetto E	1	3.226
Bertagna S	1	3.226
Bucci V	1	3.226
Buche P	1	3.226
Busset G	1	3.226
Cai JR	1	3.226
Cashman SA	1	3.226
Celebi AD	1	3.226
Cooper J	1	3.226
Cozzarini L	1	3.226
Davis CB	1	3.226
De Faria ABB	1	3.226
De Koning D	1	3.226
Destercke S	1	3.226

Edelen AN	1	3.226
Ensinas AV	1	3.226
Fischer U	1	3.226
Fleitmann L	1	3.226
Gani R	1	3.226
Gillani S	1	3.226
Guest JS	1	3.226
Hauner I	1	3.226
Hawkins TR	1	3.226
Heer PK	1	3.226
Helmdach D	1	3.226
Hilty LM	1	3.226
Ingwersen W	1	3.226
Janowicz K	1	3.226
Jolliet O	1	3.226
Kalakul S	1	3.226
Keller AA	1	3.226
Kroger L	1	3.226
Lapkin AA	1	3.226
Laurini E	1	3.226
Le Lann JM	1	3.226
Longo G	1	3.226
Malakul P	1	3.226
Marino A	1	3.226
Mery Y	1	3.226
Mio A	1	3.226
Moore G	1	3.226
Morales-mendoza LF	1	3.226
Mutel C	1	3.226
Mutel CL	1	3.226
Norris GA	1	3.226
Ouattara A	1	3.226
Paulsen H	1	3.226
Perrenoud M	1	3.226
Prioux N	1	3.226
Qu S	1	3.226
Randall PM	1	3.226
Reinhard J	1	3.226
Rerat C	1	3.226
Rivela B	1	3.226
Ruiz-mercado G	1	3.226
Ruiz-mercado GJ	1	3.226
Scanlon K	1	3.226
Schweidtmann AM	1	3.226
Sharma S	1	3.226
Shi R	1	3.226
Siemanond K	1	3.226
Song RS	1	3.226
Sperandio M	1	3.226
Srocka M	1	3.226
Steubing B	1	3.226
Suh S	1	3.226
Tiruta-bama L	1	3.226
Tiruta-barna L	1	3.226
Tock L	1	3.226
Toma L	1	3.226
Transue TR	1	3.226
Yaseneva P	1	3.226
Zah R	1	3.226
Zhu J	1	3.226

Table S3. Empirical Analysis of Reviewed Papers.

Data Source	Nr.	Literature Source	Short Description	Examples/Case Studies	Used after publication	Topic	Code/Software are freely available	parameter uncertainty	Uncertainty method	Automation Method	University/Employer	Country First Author	Journal	Publisher
Plant Data	1	Pereira et al. 2013 [3]	Shortcut Model for Standard Operating Procedure	Steam consumption of two factories in Switzerland using their standard operating procedures (SOPs) [3]	not found	chemical production	x	✓	fuzzy intervals	standard process documentation, rules of thumb, expert opinion, and thermodynamic principles.	ETH Zürich	Switzerland	Industrial & Engineering Chemistry Research	American Chemical Society
	2	Cashman et al. 2016 [4]	Data Mining from EPA	case study on acetic acid [4]; extended by Meyer et al. [5] for a case study on cumene manufacturing	yes [5]	chemical production	x	✓	Data quality analysis,Monte Carlo	data mining and linked open data	Eastern Research Group	USA	Environmental Science & Technology	American Chemical Society
LCA Databases	3	Reinhard et al. 2016 [6]	LCI database developer's prioritization	Ecovinent update [7]	yes	general	x	x		contribution-based prioritization method	University of Zurich	Switzerland	The International Journal of Life Cycle Assessment	Springer
	4	Ingwersen et al. 2015 [8]	New data architecture	Federal LCA Commons [9]	yes [9]	✓	x		Contribution analysis	Resource Description Framework - making different database with different data formats relateable	US Environmental Protection Agency	USA	The International Journal of Life Cycle Assessment	Springer
	5	Mittal et al. 2018 [10]	sementic data methodology for automated inventory modelling	nylon-6 production [10]	not found	chemical production	x	x		resource description frame- work	US Environmental Protection Agency	USA	Sutainable Chemistry & Engineering	American Chemical Society
	6	Steubing and de Koning 2021 [11]	Superstructure for future scenarios in background data	electric vehicles using future background scenarios for	not found	general	upon request	x		superstructure process management	Leiden University	Netherlands	The International Journal of Life Cycle	Springer

				from 2020 to 2050 [11]									Assessment	
	7	Ingwersen, Kahn, and Cooper 2018; Srocka 2019 [12,13]	Bridge processes – autoprox	Presented and discussed in Kuczenski et al. [14]; not used in a LCA	not found	general	upon request	x		Automated Bridge processes creation by a code written in Kotlin, to connect fore- and background data	US Environmental Protection Agency	USA	The International Journal of Life Cycle Assessment	Springer
	8	Kuczenski et al. 2016, 2021 [14,15]	Connection from data and different data sources	Olca: Example for parametrized process [16]	not found	general	✓	x		different solutions for connecting data sources using techniques like web scraping, Mock values or classification via metadata search	University of California	USA	The International Journal of Life Cycle Assessment	Springer
Scientific Literature	9	Belaud et al. 2021; Lousteau-Cazalet et al. 2016; Prioux et al. 2021 [17–20]	Knowledge Engineering (KE) for data extraction	sugar yield after enzymatic hydrolysis [20]; pretreatment processes of rice straw and corn stover [18,19,21]	original model from 2016 was further developed	Biorefinery	x	✓	pedigree matrix	KE methods	Université de Toulouse	France	Waste and Biomass Valorization	Springer
Process Simulation	10	Fermeglia, Longo, and Toma 2008; 2009 [22,23]	Process Sustainability Prediction Framework for Cape Open	phthalic anhydride from naphthalene [22]; Maleic Anhydride Production Process [23]	No, but (Morales-Mendoza et al. [24] refers to it as wanting to extend it	chemical production	upon request	x		Visual Basic based framework interacting through Cape Open with process simulation software (PROII, Aspen Plus, COCO/COFE).	University of Trieste	Italy	Environmental and Energy Engineering	American Institute of Chemical Engineers
	11	Morales-Mendoza et al. 2018	Ecodesign Framework	benzene production and biodiesel production process from waste	yes [25]	Biorefinery, Food production	x	x		automated coupling framework, the Ecodesign Framewor	ETH Zurich	Switzerland	Energy & Environmental Science	Royal Society of Chemistry

			vegetable oil [24]; milk evaporation process [25];						k, used with process simulation software COCO, ProSim Plus, and Aspen HYSYS.				
12	S. T. Gillani 2013; S. Gillani et al. 2013 [24,26,27]	SimLCA	Jatropha biodiesel production system [26,27]	not found	Biorefinery	x	✓	pedigree matrix	automated updating of simulation ProSim Plus data in their own developed LCA software	Laboratoire de Génie Chimique	France	CHEMICAL ENGINEERING TRANSACTIONS	Italian Association of Chemical Engineering
13	Busset, Belaud, and Montréjaud-Vignoles 2014; Busset et al. 2015 [21,28]	process-product-enterprise (P²E) and &cOlive	Olive oil production [28]	No, although two of the authors developed SimLCA, so knowledge is probably transferred from it	Food production	x	~	"uncertainty analysis is partially proposed"	developed VBA application converting data directly from process simulation to a product model and for sustainability assessment.	Université de Toulouse	France	CHEMICAL ENGINEERING TRANSACTIONS	Italian Association of Chemical Engineering
14	Celebi et al. 2017 [29]	thermo-environomic optimization methodology	Wood to product (sugars and syngas) [29]	not found	Biorefinery	upon request	x		data obained by Aspen Plus and Belsim VALI were combined and used for LCA calculation; the MILP problem was solved by the Lua-OSMOSE framework	Ecole Polytechnique Federale de Lausanne	Switerzland	Energy	Elsevier
15	Mery et al. 2013 [30]	simulation tool for water treatment EVALEAU	drinking water plant located in the Paris region [30]	used data and EVALEAU software [31]	water treatment processes	x	x		data from the water treatment simulation tool EVALEAU and calculations from the	Université de Toulouse	France	The International Journal of Life Cycle Assessment	Springer

										water chemistry calculation software PHREEQC were via a python code imported into the LCA Software Umberto.				
	16	Bisinellae Faria et al. 2015 [32]	DM-LCA approach	different treatment options for Urine Source-Separation [32]	not found	Water treatment processes	x	x		coupling the software BioWin through a python script with LCA in Umberto	Université de Toulouse	France	Water Research journal	Elsevier
	17	Gonzalez-Garay and Guillen-Gosalbez 2018 [33]	SUStainable ChemicAl ProcEsses (Suscape) Framework	production of methanol from CO_2 and hydrogen [33,34]; production of methanol with H2 derived from fossil fuels compare it with 10 alternative transportation liquid fuels [34]	yes, [34]	chemical production	x	x		automated connection between Aspen-HYSYS and LCA missing; usage of surrogate modelling, objective reduction, multi-objective optimization and data envelopment analysis (DEA)	Imperial College London	UK	Chemical Engineering Research and Design	Elsivier
	18	Kalakul et al. 2014 [35]	LCSoft	bioethanol production process using cassava rhizome [35,36]	yes [36,37]	process desing	x	✓	Monte Carlo analysis	LCA Software LCSoft which can interact with other software like one for sustainable design (SustainPro) or economic analysis (ECON)	Technical University of Denmark	Denmark	Journal of Cleaner Production journal	Elsevier
	19	Helmdach et al. 2017 [38]	Process Optimization with gProms,	conversion of terpenes derived from biowaste feed- stocks	not found	biorenewable-based energy; chemical productio	x	x		automated connection between the process simulation	University of Cambridge	UK	ChemSusChem	Chemistry Europe

			Matlab and Umberto	into reactive intermediates [38]						software gPROMS, the LCA-software Umberto and MATLAB. TS-EMO algorithm for optimization				
	20	Tock, Maréchal, and Perrenoud 2015 [39]	thermo-environomic model	ammonia production [39]	not found	chemical production	x	x		Integration of LCA as a function in the process simulation software Belsim Vali4, optimization done with evolutionary algorithm	Ecole Polytechnique Federale de Lausanne	Switerzland	The Canadian Journal of Chemical Engineering	The Canadian Society for Chemical Engineering
	21	Shi and Guest 2020; Cortes-Peña et al. 2020 [40,41]	BioSTEAM	sugarcane ethanol production [40], co-production of biodiesel and ethanol from lipid-cane and the production of second-generation ethanol from corn stover [41], actic acid production from lignocellulosic biomass [42], renewable linear alpha-olefins by base-catalyzed dehydration of biologically-derived fatty alcohols [43]	Yes, [42,43]	biorefinery	✓	✓	Monte Carlo analysis	integrated LCA based on Brightway in process simulation software (automation in data transfer)	University of Illinois at Urbana-Champaign	United States	Sutainable Chemistry & Engineering	American Chemical Society
Process Calculations	22	Kleinekorte et al. 2019 [44]	ANN for Molecular & Process Descriptors	CO_2- & fossilbased production of methanol	not found	chemical production	x	x		artificial neural network	RWTH Aachen	Germany	Computer Aided Chemic	Elsevier

				and formicacid [44]							University		al Engineering	
Stoichiometry	23	Pereira et al. 2018 [45]	Statistical Models Based on Reaction Synthesis	Energy consumption via Classification tree & Probability Density Function (PDF) Model [45]	not found	chemical production	x	✓	Monte Carlo simulation	probability density functions (PDF) and classification trees	ETH Zurich	Switzerland	Sutainable Chemistry & Engineering	American Chemical Society
Molecular Structure Models	24	Wernet et al. 2009; 2008 [46,47]	FineChem model (R-Package)	petrochemical field ("Fine Chem – Safety and Environmental Technology Group ∣ ETH Zurich" n.d.; [48]; postcombustion on CO2 capture [49]; bio-based production of platform chemicals [50,51]; Soft PVC plastic and a tobacco flavor [52]	yes (see examples)	chemical production	✓	✓	individual standard deviation	artificial neural network	ETH Zurich	Switzerland	Green Chemistry	The Royal Society of Chemistry 2009
	25	Song, Keller, and Suh 2017 [53]	Predictive LCIA-Model for Organic Chemicals	Case studies on acetic anhydride & hexafluoroethane [53]	not found	chemical production	✓	✓	Euclidean distance-based AD measurement	artificial neural network	University of California	USA	Environmental Science and Technology	American Chemical Society
	26	Kleinekorte et al. 2020 [54]	ANN vs. Gaussian Process Regression	yes, but training data reference was not visible [54]	not found	chemical production	x	x		artificial neural network, Gaussian Process Regression	RWTH Aachen University	Germany	Conference Book	AIChE Annual Meeting 2020
	27	Meyer et al. 2019 [5]	Purpose-Driven Reconciliation for estimating chemical production release	cumene production [5]	not found	chemical production	✓	x		Classification and Regression Tree, Random Forest	U.S. Environmental Protection Agency	USA	Sutainable Chemistry & Engineering	American Chemical Society
	28	Hou et al. 2020 [55]	machine learning models for estimating ecotoxicity	Estimation of HC50 and CFeco [55]	not found	chemical production	x	✓	confidence interval and cook's distance measures	Radom Forest	University of Michigan	USA	Environment International journal	Elsevier

			characterization factors											
	29	Mio et al. 2021 [56]	Multiscale modelling techniques in life cycle assessment	nano-engineered thermoplastic polymers Mio et al. 2021	not found	nano material production	x	x		lack on details	University of Trieste	Italy	Sustainable Materials and Technologies	Elsevier
Proxy	30	Hou et al. 2018, Xu et al. 2021 [57,58]	Similarity-Based Approach	on the UPR dataset in the ecoinvent 3.1 default model (Hou et al. 2018 [55]), (Xu et al. 2021 [58])	not found	general	✓	✓	confidence intervals using bootstrapping	similarity-based link prediction method	University of Michigan	USA	Environmental Science and Technology	American Chemical Society

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