Electronic Supplementary Material (ESI) for RSC Sustainability.

Supplementary material

"Biosurfactants' production with substrates from sugar industry - Environmental, cost, market, and social aspects"

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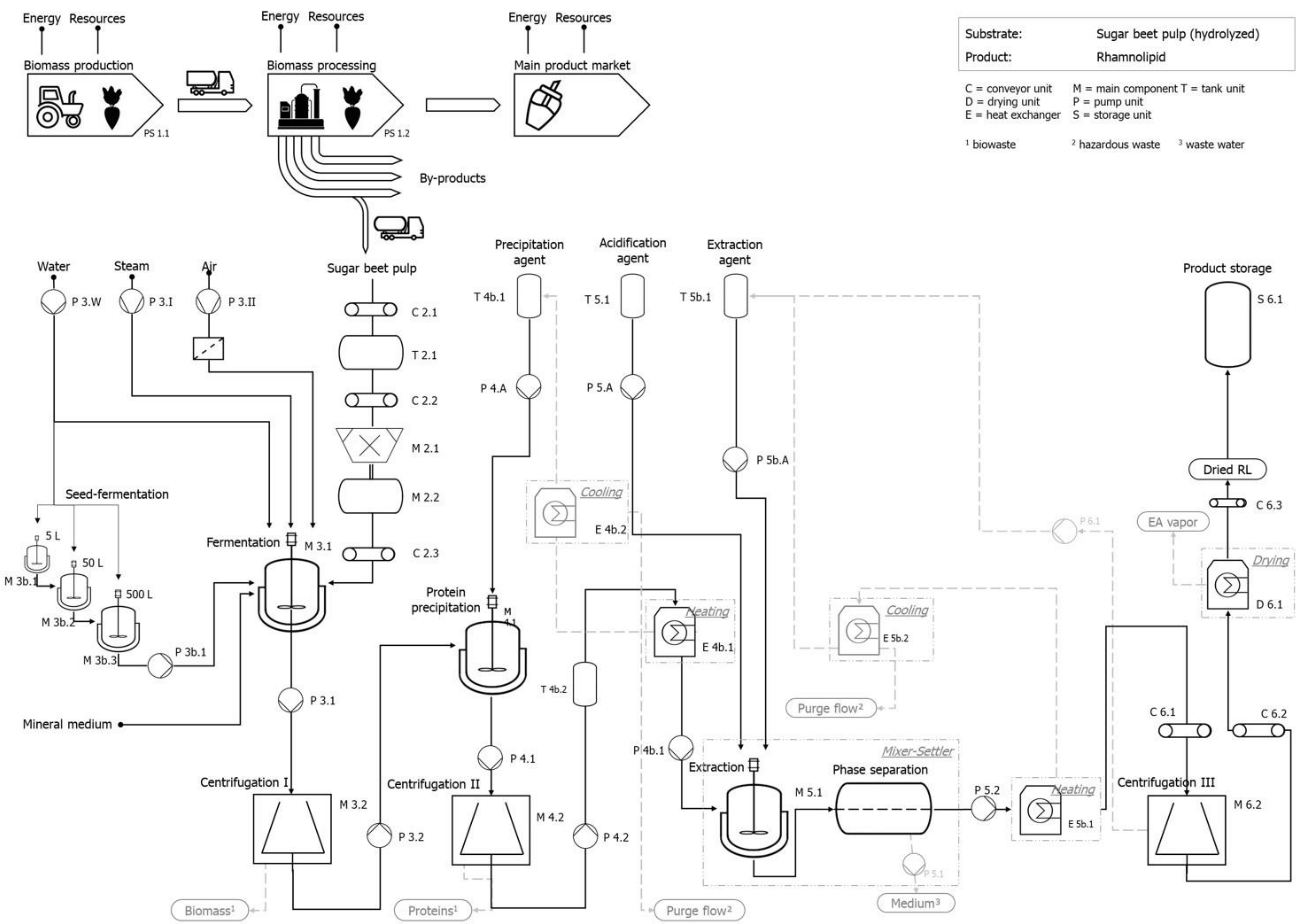
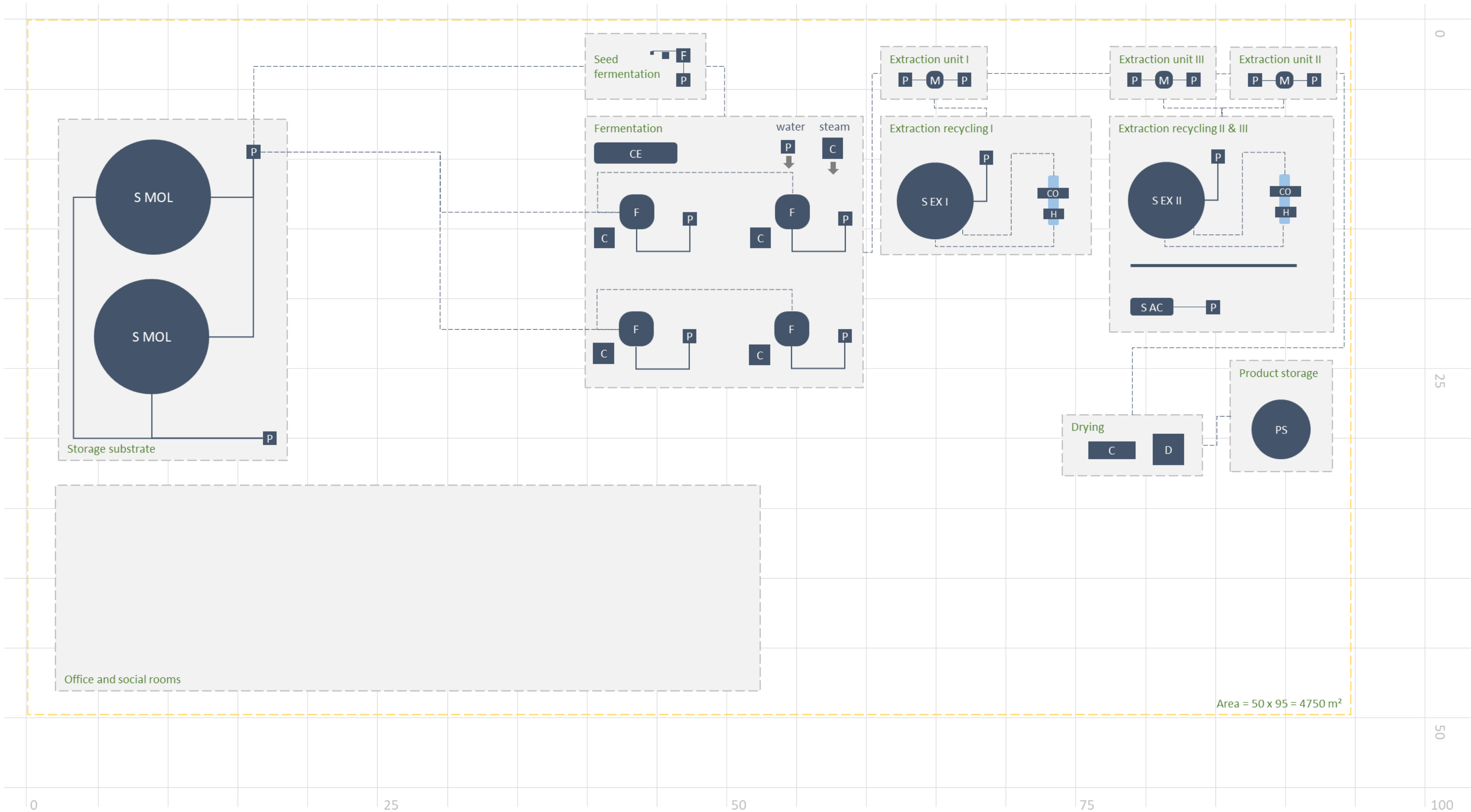
I. Additional figures and tables

Process flow chart



Supplementary Figure S1: Exemplary simplified illustration of the biosurfactant production process for the production of rhamnolipids with sugar beet pulp with description of specific process stages and modules.



Substrate:	Molasses
Product:	MEL

C = conveyor unit
CE = centrifugation unit
CO = cooling unit
D = drying unit
E = heat exchanger

F = fermentation / seed fermentation
H = heating unit
M = mixer settler unit
P = pump unit
S AC = storage acidification agent

S EX = storage extraction agent
S MOL = storage molasses
PS = product storage unit
T = tank unit

Supplementary Figure S2: Exemplary simplified illustration of the plant setup of mannosylerythritol lipids production with molasses with basic component description modules for a scaled graphical estimation of the required space.

Allocation data

Supplementary Table S1: Underlying used data for the allocation in the sugar beet production and processing stage with data from Spoerri et al. (2014) and updated pricing of specific flows.

Flow type		Main product and Co-products	Amount	Dry matter content	Economic value			Share of econ. value	Relevant for allocation	Source / comment
			[kg/t_{sugar}]	[%]	[€/Mg]	[€/kg]	[€]	[%]		
in	material flow	Sugar beet	6,800.0		28.00	0.03				LBLUEN (2019), price of Nordzucker AG for 2020
out	material flow	White granulated sugar	1,000.0	1.00	404.00	0.40	404.00	64.26		EU reference price, EU AGRI G4 (2020)
out	material flow	Beet soil	750.2	0.69	0.00	0.00	0.00	0.00		Spoerri et al. (2014), option of spreading as fertilizer
out	material flow	Sand/stones	71.7	1.00	0.00	0.00	0.00	0.00		Spoerri et al. (2014), in principle option of usage as road building material
out	material flow	Carbonatation lime	224.1	0.65	16.86	0.02	3.78	0.60		current average price from own market research
out	material flow	Wet pulp	4.3	0.11	0.00	0.00	0.00	0.00		Spoerri et al. (2014)
out	material flow	Pressed pulp	959.1	0.26	20.30	0.02	19.47	3.10		Spoerri et al. (2014); no essential pricing change
out	material flow	Dried pulp w. molasses	132.0	0.94	200.00	0.20	26.40	4.20	X	current average price from own market research
out	material flow	Dried pulp w. vinasse & raffin.	31.1	0.88	200.00	0.20	6.22	0.99	X	current average price from own market research
out	material flow	Molasses	134.1	0.80	200.00	0.20	26.82	4.27	X	current average price from own market research
out	material flow	Betaine	4.9	0.55	884.50	0.88	4.33	0.69		Spoerri et al. (2014); no essential pricing change
out	material flow	Bioethanol	151.5	0.00	900.00	0.90	136.35	21.69		assumption based on current pricing FOB Rotterdam (ca. 700 €/m³)
			[kWh]	[kg_{SKE}]*	[€/Mg_{SKE}]*		[€]			
out	energy flow	Surplus electricity	57.2	7.04	50.00		0.35	0.06		current price from own market research for energy prices
out	energy flow	Surplus heat	163.2	20.07	50.00		1.00	0.16		current price from own market research for energy prices
		total			2,925.66		628.73	100.00		

* SKE = coal unit

Calculation of costs

Following the calculation structure of Peters et al.[1], it is possible to estimate the total capital investment cost and total production cost based on the equipment cost derived from a parts list for each process chain. As an example, the following Supplementary Table S1 provides an overview of considered equipment positions and the equipment cost per process stage. These calculations contain additional interim results on direct costs, indirect costs, working capital, manufacturing costs, and general expenses (see Supplementary Table S2). Some cost items included in the calculation were determined by separate calculations (e.g., depreciation, labor costs), other by the use of averaged or adjusted relative values for specific cost items (e.g., piping, legal expenses, maintenance) like it is displayed in Table S2. According to Peters et al. the used relative data is applicable to "ordinary chemical processes" and can vary depending on factors like the plant location, type of process, complexity of instrumentation, and company policies.

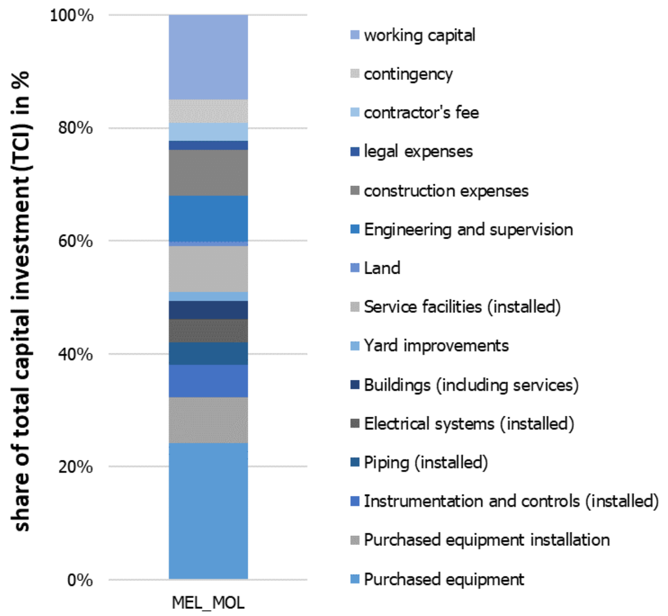
As an additional included position in Supplementary Table S2, the end-of-life (EoL) costs were estimated by the use of different calculation tools and literature based on own process-chain specific calculations of the necessary plant site layout (necessary dimensions of buildings and site for 15,000 $kg_{product}/a$). The determined costs were added in the pricing under the assumption of an area use for 40 years.

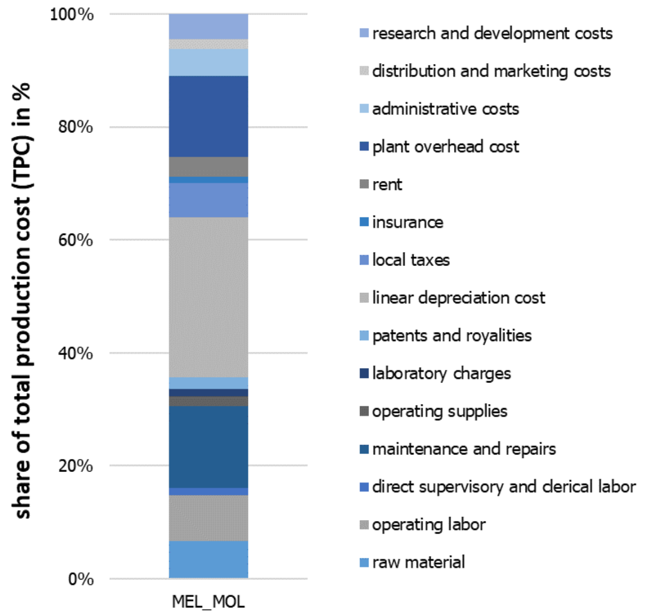
[1] Peters, M. S., Timmerhaus, K. D., & West, R. E. (2003). Plant Design and Economics for Chemical Engineers: McGraw-Hill Education.

Supplementary Table S2: Underlying calculation positions for all considered process chains with calculation factors and the related reference data (based on and derived from data from Peters et al. (2003)); exemplary cost data for the MEL_MOL process chain.

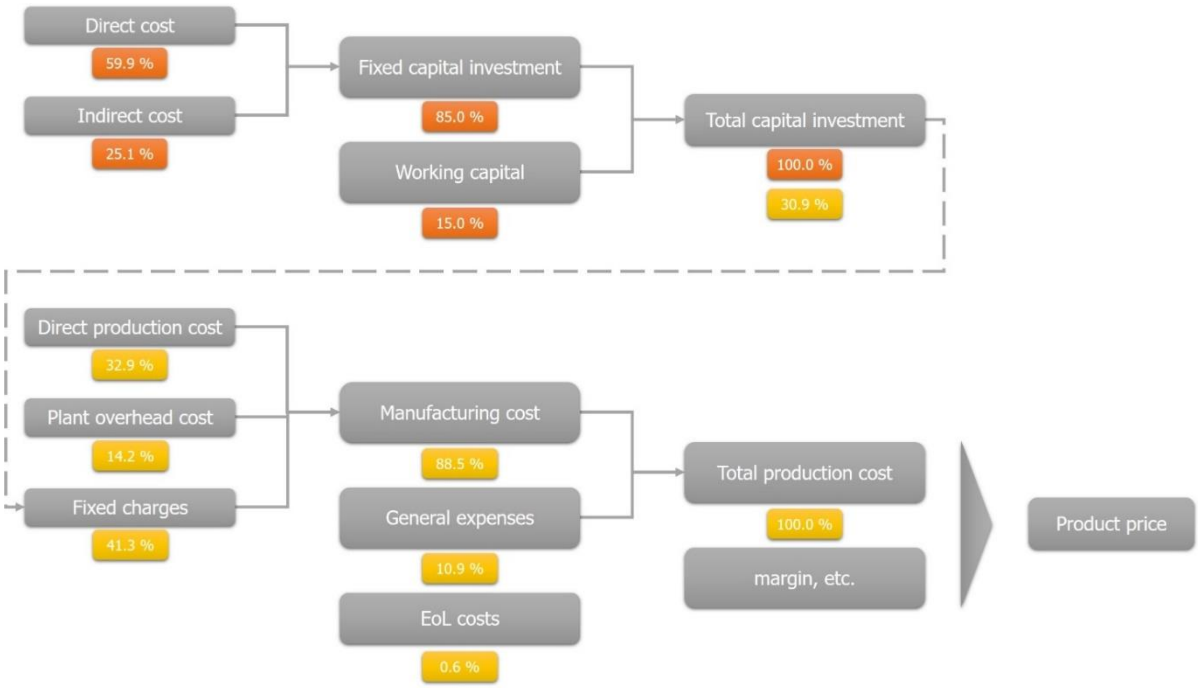
field of cost	**cost group** / cost position	calculation factor [%$_{of\ reference}$]	exemplary data for MEL_MOL value	unit	reffered to / sum of
CAPITAL INVESTMENT COST (Investment)	**direct cost**				
	Purchased equipment	28.6	3,359,706	€	own calculation
	Purchased equipment installation	9.5	1,119,902	€	purchased equipment
	Instrumentation and controls (installed)	6.7	783,931	€	purchased equipment
	Piping (installed)	4.8	559,951	€	purchased equipment
	Electrical systems (installed)	4.8	559,951	€	purchased equipment
	Buildings (including services)	3.8	447,961	€	purchased equipment
	Yard improvements	1.9	223,980	€	purchased equipment
	Service facilities (installed)	9.5	1,119,902	€	purchased equipment
	Land	1.0	111,990	€	purchased equipment
	indirect cost				
	Engineering and supervision	9.5	1,119,902	€	purchased equipment
	construction expenses	9.5	1,119,902	€	purchased equipment
	legal expenses	1.9	223,980	€	purchased equipment
	contractor's fee	3.8	447,961	€	purchased equipment
	contingency	4.8	559,951	€	purchased equipment
	fixed Capital Investment		11,758,970	€	direct cost + indirect cost
	working capital	15	2,075,112	€	Fixed capital investment
	total capital investment		13,834,083	€	fixed capital investment + working capital
	depreciation time [y]	10 y			
TOTAL PRODUCTION COST (Operation)	**direct production cost**		1,738,630		
	raw material	-	327,759	€/a	own calculation
	operating labor	-	397,800	€/a	own calculation
	direct supervisory and clerical labor	15	59,670	€/a	operating labor
	maintenance and repairs	6	705,538	€/a	fixed capital investment
	operating supplies	0.75	88,192	€/a	fixed capital investment
	laboratory charges	15	59,670	€/a	operating labor
	patents and royalities	2	100,000	€/a	assumption
	fixed charges		1,907,177	€/a	
	linear depreciation cost	-	1,383,408	€/a	own calculation from total capital investment
	local taxes	2.5	293,974	€/a	fixed capital investment
	insurance	0.5	58,795	€/a	fixed capital investment
	rent	8	171,000	€/a	own calculations
	plant overhead cost	60	697,805	€/a	operating labor, direct supervisory and clerical labor, maintenance and repairs
	Manufacturing cost	sum	4,343,612	€/a	direct production cost + fixed charges + plant overhead cost
	general expenses		536,654	€/a	
	administrative costs	20	232,602	€/a	operating labor, direct supervisory and clerical labor, maintenance and repairs
	distribution and marketing costs	2	86,872	€/a	manufacturing cost
	research and development costs	5	217,181	€/a	manufacturing cost
	total production cost	sum	4,880,267	€/a	manufacturing cost + general expenses
FOLLOWING COST	**following cost**				
	total following costs (EoL)	-	1,073,402	€	own calculations
	specific following costs (EoL)	-		€/a	own calculations
	End of Life time [y]	40 y			assumption
	total production cost + EoL cost	sum	4,907,102	€/a	total production cost + EoL cost
PRICING	**pricing**				
	minimum price (incl. EoL cost)	-			own calculations

Derived from the data in Supplementary Table S2 the following figures show the shares of cost positions on total capital investment (TCI) and total production cost (TPC).





As shown in the following Supplementary Figure S3, the cost calculations of the products in the present study are based on a cost estimation for “total capital investment” and “total production cost” (including EoL cost). The total capital investment (TCI) is mainly determined by the fixed capital investment (85%TCI), which is calculated by direct (59.9%TCI; e.g., equipment costs, building or electrical system costs) and indirect costs (25.1%TCI; e.g., engineering costs or legal expenses). The total production costs (TPC) comprise the dominating manufacturing costs (88.5%TPC; e.g., raw materials, laboratory charges, or linear depreciation costs), the general expenses (10.9%TPC; e.g., administrative or marketing costs), and EoL costs (< 1%TPC; EoL cost). The manufacturing costs are divided into direct production costs (32.9%TPC), plant overhead costs (14.2%TPC), and fixed charges (41.3%TPC, thereof 30.9% connected to the TCI). The percentage data are to be interpreted in the corresponding color context (green or yellow) and refer to the items marked with 100% in each case. Additional factors such as CO2-pricing, if necessary, margins, and others have to be added to calculate a selling price.



Supplementary Figure S3: Exemplary cost and pricing structure with relative shares of total capital investment (orange colored), total production cost (yellow colored), and the product price including margin, etc. for MEL production with SBP.

Supplementary Table S3: Underlying cost positions for equipment costs of the process chain MEL_MOL for annual production of 15,000 kg product including costs per process stage, contained process modules and number of items.

position no.[1]	process stage	process module	number of items	equipment cost per process stage[2]	source of equipment cost[2]
			-	€	-
PS 1.1 PS 1.2	Sugar beet production and processing	- -	- -	covered by purchase price	
P 2.1 T 2.1 P 2.2	Storage and preparation	pump molasses storage tank molasses pump molasses	1 2 1	266,538	● cost research via: alibaba.com matche.com
M 3.1 P 3.1 M 3.2 P 3.2 P 3.W P 3.I P 3.II - -	Fermentation	fermentation tank pump fermentation broth centrifugation unit I pump fermentation broth liquids pump water compressor steam compressor air + filter stirrer membrane	4 4 1 4 1 1 4 4 4	1,845,722	● cost calculations based on Knoll (2008)[3] ● cost research via: alibaba.com matche.com mixerdirect.com ● information from project partners
M 3b.1 M 3b.2 M 3b.3 P 3b.1 -	Seed fermentation	fermenter 5 L fermenter 50 L fermenter 500 L pump fermentation medium stirrer	1 1 1 1 3	102,208	● cost research via: alibaba.com matche.com mixerdirect.com ● estimations
M4.1 P 4.1 P 4.2	Extraction 01	mixer settler unit I pump extraction agent recycling pump broth residue	1 1 1	207,670	● cost research via: alibaba.com matche.com
T 4b.1 P 4b.A E 4b.1 E 4b.2 C 4b.1	Extraction recycling I (included in Extraction 01)	extraction agent tank pump extraction agent extraction agent heating unit extraction agent cooling unit conveyor unit IV	1 1 1 1 1	219,655	● cost research via: alibaba.com eurolux-ag.com ● estimations
T 4c.1 T 4c.2 P 4.A P 4c.A1 P 4c.A2 E 4c.3 E 4c.4	Extraction recycling II & III (included in Extraction 02 & 03)	extraction agent 2 tank acidification agent 2 tank pump acidification agent pump extraction agent pump extraction agent extraction agent cooling unit II extraction agent heating unit III	1 1 1 1 1 1 1	193,114	● cost research via: alibaba.com matche.com eurolux-ag.com ● estimations
M 4.2 P 4.3 P 4.4	Extraction 02	mixer settler unit II pump extraction agent recycling pump broth residue	1 1 1	202,000	● cost research via: alibaba.com matche.com
M 4.3 P 4.5 P 4.6	Extraction 03	mixer settler unit III pump extraction agent recycling pump broth residue	1 1 1	202,000	● cost research via: alibaba.com matche.com
M 5.1 D 5.1 C 5.1 C 5.2 S 5.1	Final conditioning	centrifugation unit II drying unit conveyor unit VII conveyor unit VIII product storage	1 1 1 1 1	120,800	● cost research via: matche.com ● estimations
		total		***3,359,706***	

[1] related to flow chart
[2] data status: 2021
[3] inflation included

Results LCA Contributions

Supplementary Table S4/1: LCIA results for the most contributing process modules and flows (per impact category) of RL production in the context of the six most contributing impact categories (to total impact) per considered process chain; share of impact categories impact on total impact per process chain.

impact category	share of impact category on total impact (range of process chains)	RL_MOL share of impact category on total impact %	RL_MOL share of contributing flow on total impact of specific category %	RL_MOL mainly responsible process module of origin	RL_MOL share of contributing process module on total impact of specific category %	RL_SBP share of impact category on total impact %	RL_SBP share of contributing flow on total impact of specific category %	RL_SBP mainly responsible process module of origin	RL_SBP share of contributing process module on total impact of specific category %
ecotoxicity freshwater - total	21-30 %	22.3				20.8			
most contributing flows (overall)		*chloride*	26.8	treatment of hazardous waste [PAR]	9.3	*chloride*	27.8	treatment of hazardous waste [PAR]	11.5
		sulphur	22.7	pottasium chloride production [SBPP]	21.5	*hydrogen sulphide*	18.2	treatment of biowaste [FER]	11.3
resource use, fossils	19-26 %	24.7				25.8			
most contributing flows (overall)		*gas, natural, in ground*	30.7	acetone production [PAR]	25.8	*gas, natural, in ground*	31.6	acetone production [PAR]	28.0
		crude oil ecoinvent	26.3	acetone production [PAR]	19.3	*crude oil ecoinvent*	26.4	acetone production [PAR]	20.9
climate change - total	9-11 %	10.5				10.9			
most contributing flows (overall)		*carbon dioxide*	84.2	acetone production [PAR]	26.3	*carbon dioxide*	84.6	acetone production [PAR]	28.7
		methane	13.1	acetone production [PAR]	9.2	*methane*	13.5	acetone production [PAR]	10.0
eutrophication, freshwater	5-6 %	5.6				5.1			
most contributing flows (overall)		*phosphate*	48.5	treatment of hazardous waste [PAR]	18.7	*phosphate*	53.2	treatment of hazardous waste [PAR]	23.1
		phosphorus	39.4	acetone production [PAR]	18.6	*phosphorus*	37.0	acetone production [PAR]	22.8
acidification	4-6 %	5.8				6.0			
most contributing flows (overall)		*sulphur dioxide*	39.5	acetone production [PAR]	34.9	*sulphur dioxide*	41.9	acetone production [PAR]	38.0
		nitrogen oxides	15.1	acetone production [PAR]	13.2	*nitrogen oxides*	15.9	acetone production [PAR]	14.4
resource use, minerals and metals	3-6 %	3.0				2.8			
most contributing flows (overall)		*tellurium*	47.4	ethyl acetate production [EX]	28.7	*tellurium*	44.9	ethyl acetate production [EX]	21.9
		chromium	17.6	steel production [FER]	5.1	*chromium*	22.5	steel production [FER]	5.8
share of six impact categories on total impact		71.9				71.5			
average share of process module on total impact of specific category					*19.2*				*19.7*

EX = Extraction; EX 01 = Extraction #1; FER = Fermentation; PAR = Precipitation Agent Recovery; SBPP = Sugar beet production and processing

Supplementary Table S4/2: LCIA results for the most contributing process modules and flows (per impact category) of MEL production in the context of the six most contributing impact categories (to total impact) per considered process chain; share of impact categories impact on total impact per process chain.

impact category	share of impact category on total impact (range of process chains)	MEL_MOL share of impact category on total impact %		share of contributing flow on total impact of specific category %	mainly responsible process module of origin	share of contributing process module on total impact of specific category %	MEL_SBP share of impact category on total impact %		share of contributing flow on total impact of specific category %	mainly responsible process module of origin	share of contributing process module on total impact of specific category %
ecotoxicity freshwater - total	21-30 %	29.5					28.5				
most contributing flows (overall)			*sulphur*	21.1	pottasium chloride production [SBPP]	19.6		*chloride*	19.9	treatment of hazardous waste [EX 01]	3.8
			chloride	20.9	pottasium chloride production [SBPP]	4.9		*aluminium*	19.2	ethyl acetate production [EX 01]	11.4
resource use, fossils	19-26 %	18.8					19.5				
most contributing flows (overall)			*crude oil ecoinvent*	21.9	ethyl acetate production [EX 01]	13.8		*crude oil ecoinvent*	22.1	ethyl acetate production [EX 01]	14.6
			natural gas	19.3	compressed air supply [FER]	7.3		*natural gas*	16.8	compressed air supply [FER]	8.0
climate change - total	9-11 %	8.5					8.6				
most contributing flows (overall)			*carbon dioxide*	89.0	compressed air supply [FER]	27.5		*carbon dioxide*	89.8	compressed air supply [FER]	30.9
			methane	7.9	ethyl acetate production [EX 01]	4.0		*methane*	8.2	ethyl acetate production [EX 01]	4.3
eutrophication, freshwater	5-6 %	6.4					6.1				
most contributing flows (overall)			*phosphate (longterm)*	57.9	ethyl acetate production [EX 01]	16.6		*phosphate [longterm]*	64.9	ethyl acetate production [EX 01]	36.4
			phosphate	23.4	ethyl acetate production [EX 01]	16.6		*phosphate*	25.3	ethyl acetate production [EX 01]	18.8
acidification	4-6 %	4.3					4.4				
most contributing flows (overall)			*nitrogen oxides*	17.8	compressed air supply [FER]	7.2		*nitrogen oxides*	17.8	compressed air supply [FER]	8.0
			sulphur dioxide	16.8	compressed air supply [FER]	9.9		*sulphur dioxide*	17.8	compressed air supply [FER]	11.1
resource use, minerals and metals	3-6 %	5.8					6.2				
most contributing flows (overall)			*tellurium*	55.8	ethyl acetate production [EX 01]	38.5		*tellurium*	56.2	ethyl acetate production [EX 01]	39.0
			gold	13.9	ethyl acetate production [EX 01]	9.7		*gold*	13.9	ethyl acetate production [EX 01]	9.8
share of six impact categories on total impact			73.3					73.3			
average share of process module on total impact of specific category						*14.6*					*16.4*

EX = Extraction; EX 01 = Extraction #1; FER = Fermentation; PAR = Precipitation Agent Recovery; SBPP = Sugar beet production and processing

Supplementary Table S5/1: Cost data sources of material and services for the biosurfactants production cost analysis and S-LCA.

	substrate	price net [€]	price gross [€]	unit	year	supplier	source
molasses							
1	molasses	335.00	398.65	[€/Mg]	2018	Dieckmann Technik GmbH	http://www.dootec.de/melasse-ibc
2	molasses	270.00	321.30	[€/Mg]	2018	Dieckmann Technik GmbH	http://www.dootec.de/melasse-ibc
3	molasses	209.00	248.71	[€/Mg]	2017	Blatterspiel Agrarhandel e.K.	https://www.rh-agrarhandel.de/
4	molasses	199.00	236.81	[€/Mg]	2017	Blatterspiel Agrarhandel e.K.	https://www.rh-agrarhandel.de/
5	Beet molasses	128.05	152.38	[€/Mg]	2011	-	Maung, T.A. et al. 2011. The economic feasibility of sugar beet biofuel production in central North Dakota in Biomass and Bioenergy Volume 35. Issue 9. October 2011. Pages 3737-3747
6	molasses	242.14	288.14	[€/Mg]	2017	MBR Thurgau AG	www.maschinenring.ch
7	beet molasses 42 %	158.25	188.32	[€/Mg]	2011	DMH Agrar GmbH	https://www.deutsche-melasse.de/
8	beet molasses 42 %	174.53	207.69	[€/Mg]	2014	DMH Agrar GmbH	https://www.deutsche-melasse.de/
9	beet molasses 42 %	152.77	181.80	[€/Mg]	2015	DMH Agrar GmbH	https://www.deutsche-melasse.de/
ø		207.64	247.09	[€/Mg]			
used	molasses	200.00		[€/Mg]			
sugar beet pulp							
1	sugar beet pulp	147.00	174.93	[€/Mg]	2017	Rheinischen Warenbörse e.V.	https://www.rheinische-warenboerse.de/
2	sugar beet pulp	260.47	309.96	[€/Mg]	2012	-	Losand, B. (2012) Sächsischer Futtertag 2012, Protein aus Nebenprodukten
3	dry sugar beet pulp	172.60	205.39	[€/Mg]	2017	Landwirtschaftskammer Schleswig-Holstein	http://www.lksh.de/landwirtschaft/betriebswirtschaft-beratung/markt/futtermittel/ Preisliste
4	dry sugar beet pulp pellets	170.00	202.30	[€/Mg]	2018	WVZ e.V.	https://www.zuckerverbände.de
5	dry sugar beet pulp	220.00	261.80	[€/Mg]	2017	DMH Agrar GmbH	https://www.deutsche-melasse.de/
6	dry sugar beet pulp	147.00	174.93	[€/Mg]	2017	DMH Agrar GmbH	https://www.deutsche-melasse.de/
ø		186.18	221.55	[€/Mg]			
used	sugar beet pulp	200.00		[€/Mg]			

Supplementary Table S5/2: Cost data sources of material and services for the biosurfactants production cost analysis and S-LCA.

	substrate	price net [€]	price gross [€]	unit	year	supplier	source
water							
1	tap water	1.68	1.80	[€/m³]	2018	Gelsenwasser AG	https://www.gelsenwasser.de/wasser/preise/
2	tap water	1.84	1.97	[€/m³]	2018	Gelsenwasser AG	https://www.gelsenwasser.de/wasser/preise/
3	tap water	1.83	1.96	[€/m³]	2018	Stadtwerke Konstanz GmbH	https://www.stadtwerke-konstanz.de/energie-und-wasser/trinkwasser/allgemeiner-wassertarif/
4	tap water	1.78	1.91	[€/m³]	2018	BS|ENERGY, Braunschweiger Versorgungs-AG & Co. KG	https://www.bs-energy.de/geschaeftskunden/service/wasser/
5	tap water	1.69	1.81	[€/m³]	2018	Berliner Wasserbetriebe	http://www.bwb.de/content/language1/html/204.php
6	tap water	1.53	1.64	[€/m³]	2018	Stadtwerke Rosenheim GmbH & Co. KG	https://www.swro.de/versorgung/wasser/preise.html
7	tap water	1.74	1.86	[€/m³]	2018	Stadtwerke Kiel AG	https://www.stadtwerke-kiel.de/swk/de/produkte/privatkunden/wasser/tarife/wassertarife.jsp
8	tap water	1.25	1.34	[€/m³]	2018	Stadtwerke Emden GmbH	https://stadtwerke-emden.de/wasser/preisuebersicht/
9	tap water	2.08	2.23	[€/m³]	2018	MVV Energie AG	https://www.mvv.de/energie/gewerbe/wasser/preise-bedingungen/
10	tap water	2.00	2.14	[€/m³]	2018	Aschaffenburger Versorgungs-GmbH	http://www.stwab.de/Energie-Wasser/Wasser/Wassertarife/
Ø		1.74	1.87	[€/m³]			
used	tap water	2.00		[€/m³]			
Seed Fermernter Medium							
1	fermenter medium	20.00	23.8	[€/L]	2013	-	Andrew, W. (2013). Pharmaceutical Manufacturing Encyclopedia (3rd ed.): Elsevier Science.
Ø		20.00	23.80	[€/L]			
used	fermenter medium	20.00		[€/L]			
precipitation agent							
1	acetone	1,300.00	1,547.00	[€/Mg]	2019	alibaba.com	https://german.alibaba.com/product-detail/high-purity-98-acetone-ch3coch3-propanone-c3h6o-industrial-grade-for-plastic-rubber-fiber-leather-grease-60662133352.html?spm=a2700.8699010.normalList.80.2bd54b21yb8Ugd
2	acetone	2,004.86	2,385.78	[€/Mg]	2019	Dr. Felix Jäger Chemikalienhandel	chemical portal price listing 02/2019
3	acetone	1,720.00	2,046.80	[€/Mg]	2021	Dr. Felix Jäger Chemikalienhandel	https://www.chemikalienportal.de/loesemittel/aceton-1/aceton.html
4	acetone	1,225.00	1,457.75	[€/Mg]	2019	PCC Trade & Services GmbH	https://distripark.de/aceton-chem-rein-dimethylketon-propan-2-on-800-kg-ibc
5	acetone	880.00	1,047.20	[€/Mg]	2019	guidechem.com	https://www.guidechem.com/trade/pdetail3614485.html
6	acetone	1,760.00	2,094.40	[€/Mg]	2019	guidechem.com	https://www.guidechem.com/trade/pdetail3218893.html
Ø		1481.64	1763.16				
used	acetone	1,200.00		[€/Mg]			

Supplementary Table S5/3: Cost data sources of material and services for the biosurfactants production cost analysis and S-LCA.

	substrate	price net [€]	price gross [€]	unit	year	supplier	source
acidification agent							
1	sulphuric acid 96 %	421.40	501.47	[€/Mg]	2020	PCC Trade & Services GmbH	https://distripark.de/schwefelsaure-96-nettogewicht-1400-kg
2	sulphuric acid 96 %	380.38	452.65	[€/Mg]	2019	JOKORA GmbH	https://www.jokora.de/biogasanlagen/schwefelsaeure/schwefelsaeure-96-tech-1300-kg-container
3	sulphuric acid 96 %	274.69	326.88	[€/Mg]	2019	JOKORA GmbH	https://www.jokora.de/biogasanlagen/schwefelsaeure/schwefelsaeure-96-tech-1300-kg-container
4	sulphuric acid 96 %	264.00	314.16	[€/Mg]	2020	alibaba.com	https://german.alibaba.com/product-detail/un1830-sulfuric-acid-best-price-ibc-tank-jerrycan-60786047727.html?spm=a2700.8699010.normalList.19.4b7d24918g3g4w
5	sulphuric acid 96 %	347.60	413.644	[€/Mg]	2020	alibaba.com	https://german.alibaba.com/product-detail/chciw-h2so4-96-cas-9002-84-0-schwefels-ure-96--60667342302.html?spm=a2700.galleryofferlist.normalList.1.5922121885DKou&s=p
6	sulphuric acid 96 %	734.24	873.75	[€/Mg]	2019	Dr. Felix Jäger Chemikalienhandel	chemical portal price listing 02/2019
ø		403.72	480.42				
used	sulphuric acid 96 %	400.00	476.00				
extraction agent I							
1	ethyl acetate	26.00	30.94	[€/L]	2019	AlphaCrom AG	http://www.alphacrom.com/de/fluessig-fluessig-extraktion
2	ethyl acetate	1.00	1.19	[€/L]	2019	Vincentz Network GmbH & Co. KG	http://www.farbeundlack.de/Publikationen/Rohstoffreport/RohstoffReport-Online-Preisspiegel
3	ethyl acetate	2.48	2.95	[€/L]	2019	Dr. Felix Jäger Chemikalienhandel	https://www.chemikalienportal.de/loesemittel/ethylacetat-1/ethylacetat.html
4	ethyl acetate	3.60	4.28	[€/L]	2019	Dr. Felix Jäger Chemikalienhandel	https://www.chemikalienportal.de/loesemittel/ethylacetat-1/ethylacetat.html
5	ethyl acetate	30.00	35.7	[€/L]	2019	-	project information Bio²
6	ethyl acetate	35.00	41.65	[€/L]	2019	-	project information Bio²
7	ethyl acetate	2.48	2.95	[€/L]	2019	Dr. Felix Jäger Chemikalienhandel	chemical portal price listing 02/2019
8	ethyl acetate	10.75	12.79	[€/L]	2019	Bernd Kraft GmbH	https://berndkraft.de/
ø		13.91	16.56	[€/L]			
used	ethyl acetate	3.00					assumed price for larger purchase quantities

Supplementary Table S5/4: Cost data sources of material and services for the biosurfactants production cost analysis and S-LCA.

	substrate	price net [€]	gross [€]	unit	year	supplier	source
extraction agent II							
1	n-hexane	18.36	21.8484	[€/L]	2020	Carl Roth GmbH + Co. KG	https://www.carlroth.com/at/de/Chemikalien/A-Z-Chemikalien/H/n-Hexan/n-Hexan/p/000000010000 8c6800020023_de
2	n-hexane	30.40	36.176	[€/L]	2020	Thermo Fisher Scientific Inc.	https://www.fishersci.de/shop/products/n-hexane-95-extra-pure-acros-organics-4/p-2691924
3	n-hexane	27.86	33.15	[€/L]	2021	Zentrum für Energie- und Umweltstudien GmbH	https://www.restauro-online.com/epages/63807438.sf/de_DE/?ObjectPath=/Shops/63807438/Products/Z188
4	n-hexane	105.00	124.95	[€/L]	2021	Merck KGaA	https://www.sigmaaldrich.com/catalog/search?term=110-54-3&interface=CAS%20No.&N=0&mode=partialmaxfocus=product&lang=de&region=DE&focus=product&gclid=EAIaIQobChMI_JGStsCv5gIVT-R3Ch2kbwVKEAAYAvAAEgLnTvD_BwE
5	n-hexane	35.98	42.8162		2021	S3 Handel und Dienstleistungen UG	https://shop.es-drei.de/alkane/12314/n-hexan-min.-95?number=S1002140.5
6	n-hexane	1.18	1.4042		2021	alibaba.com	https://german.alibaba.com/p-detail/Price-1600477926669.html?spm=a2700.galleryofferlist.normal_offer.d_title.118c4defz1tvoe&s=p
7	n-hexane	1.32	1.57	[€/L]	2021	alibaba.com	https://german.alibaba.com/p-detail/organic-1600284680903.html?spm=a2700.galleryofferlist.normal_offer.d_title.118c4defz1tvoe
8	n-hexane	1.65	1.96	[€/L]	2021	alibaba.com	https://german.alibaba.com/p-detail/Cas-1600656906262.html?spm=a2700.galleryofferlist.normal_offer.d_title.118c4defz1tvoe
Ø		27.72	32.99	[€/L]			
used		5.00					assumed price for larger purchase quantities
disposal waste water							
1	waste water disposal	2.43	2.89	[€/m³]	2018	Abwassergesellschaft Halberstadt GmbH	http://www.awh.halberstadt.de/index.php/Abwasserentsorgung.html
2	waste water disposal	2.58	3.07	[€/m³]	2018	Stadtwerke Finsterwalde GmbH	https://www.stadtwerke-finsterwalde.de/cms/Abwasser/Satzungen/Abwasser-Satzungen/Preisblatt-Abwasserentsorgung-ab-01.01.2020.pdf
3	waste water disposal	2.43	2.89	[€/m³]	2018	Zweckverband Ostholstein	https://www.zvo.com/files/downloads/5-unternehmen/pflichtveroeffentlichungen-satzungen/abwasser/ZVO-Schmutzwasserbeseitigung_Gebuehrensatzung_2017.pdf
4	waste water disposal	2.65	3.15	[€/m³]	2018	Gemeinde Weeze	https://www.weeze.de/c12576b300525dd6/files/satzung_abwassergebuehren_kanalanschlussbeitraege_und_kostenersatz_fuer_grundstuecke_ab_2020.pdf/$file/satzung_abwassergebuehren_kanalanschlussbeitraege_und_kostenersatz_fuer_grundstuecke_ab_2020.pdf?openelement
5	waste water disposal	2.47	2.94	[€/m³]	2018	Märkischer Abwasser- und Wasserzweckverband (MAWV)	https://www.mawv.de/files/verband/satzungen/schmutzwasser/01-mawv-schmutzwassergebuehrensatzung-lesefassung.pdf
6	waste water disposal	2.75	3.27	[€/m³]	2018	Städtische Werke Magdeburg GmbH & Co. KG	https://www.sw-magdeburg.de/fileadmin/swm/Privatkunden/Abwasser/Dateien/Preisinformation_Abwasserentsorgung.pdf
7	waste water disposal	2.68	3.19	[€/m³]	2018	Gemeinde Bremerhaven	https://www.bremerhaven.de/de/verwaltung-politik/buergerservice/entsorgungsbetriebe-bremerhaven/entsorgungsbetriebe-bremerhaven-ebb.16447.html
8	waste water disposal	2.54	3.02	[€/m³]	2018	WasserZweckVerband- Malchin Stavenhagen	https://www.wzv-malchin-stavenhagen.de/abwassergebuehren/
9	waste water disposal	2.85	3.39	[€/m³]	2018	Stadt Krefeld	https://www.krefeld.de/kbk/inhalt/uebersicht-ueber-die-abwassergebuehren/
10	waste water disposal	2.92	3.48	[€/m³]	2018	Abwasserzweckverband Merseburg	https://azv-merseburg.de/fileadmin/Redaktion/user_upload/Gebuehrensatzung_ab_08.11.2018.pdf
Ø		2.63	3.13	[€/m³]			
used	waste water disposal	2.63		[€/m³]			

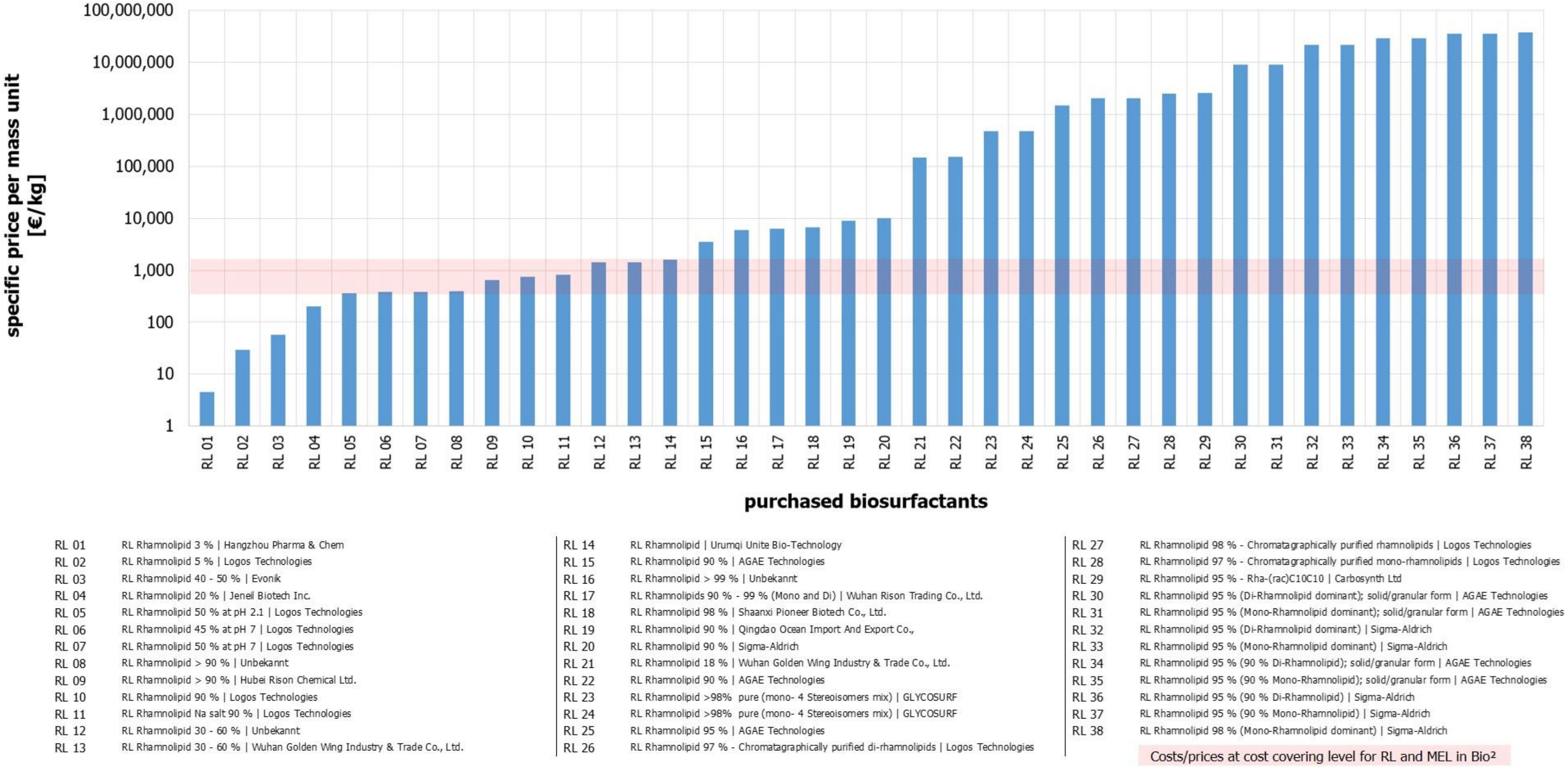
Supplementary Table S5/5: Cost data sources of material and services for the biosurfactants production cost analysis and S-LCA.

	substrate	price net [€]	price gross [€]	unit	year	supplier	source
disposal organic waste							
1	organic waste disposal	107.00	127.33	[€/m³]			https://www.eva-abfallentsorgung.de/preise-und-gebuehren.html
2	organic waste disposal	78.00	92.82	[€/m³]			www.abfallwirtschaft-vechta.de › gebuehren-preise › entsorgungspreise
3	organic waste disposal	54.05	64.32	[€/m³]			https://www.aha-region.de/fileadmin/Download/Recht/Abfallgeb%C3%BChrensatzung_01.01.2020.p
4	organic waste disposal	99.16	118.00	[€/m³]			https://www.awb-es.de/gebuehren/gewerbe/__Gewerbe-Selbstanlieferung~2.html
5	organic waste disposal	93.73	111.54	[€/m³]			https://www.abfallwirtschaft-freiburg.de/de/umschlagstation/umschlagstation.php
6	organic waste disposal	180.00	214.20	[€/m³]			https://www.egb-bir.de/fileadmin/pdf-downloads/preisblatt_egb_2018.pdf
7	organic waste disposal	191.80	228.24	[€/m³]			https://www.egb-bir.de/fileadmin/pdf-downloads/preisblatt_egb_2018.pdf
8	organic waste disposal	126.05	150.00	[€/m³]			https://www.landkreis-heidenheim.de/idc/groups/web/documents/web_asset/cms008823.pdf
9	organic waste disposal	107.39	127.80	[€/m³]			https://www.zak-kempten.de/download/aktuelle-gebuehrensatzung1.pdf
10	organic waste disposal	92.44	110.00	[€/m³]			https://www.mkw-grossefehn.de/entsorgung/entsorgungszentrum-grossefehn.html
ø		112.96	134.43	[€/m³]			
used	organic waste disposal	112.96		[€/m³]			
disposal hazardous waste							
1	solvent disposal	2.02	2.40	[€/kg]		GIB Entsorgung Wesermarsch GmbH	https://www.gib-entsorgung.de/index.php/preisliste.html
2	solvent disposal	1.55	1.84	[€/kg]		Hagener Entsorgungsbetrieb HEB GmbH	https://www.heb-hagen.de/rund-um-den-muell/muellverbrennungsanlage/gewerbe/preise.html
3	solvent disposal	1.02	1.21	[€/kg]		AWN Abfallwirtschaftsgesellschaft des Neckar-Odenwald-Kreises mbH	https://www.awn-online.de/images/downloads/merkblaetter/g10-schadstoffe_merkblatt-preisliste.p
4	solvent disposal	1.00	1.19	[€/kg]		Technische Betriebe Remscheid	https://www.tbr-info.de/entsorgungspreise.html
5	solvent disposal	1.30	1.55	[€/kg]		Technische Betriebe Remscheid	https://www.tbr-info.de/entsorgungspreise.html
6	solvent disposal	1.70	2.02	[€/kg]		Berliner Stadtreinigungsbetriebe AöR	https://www.bsr.de/abfall-abc-20563.php?fractionID=ccd0ebe5-83fc-4bb9-a913-23fbc7a58c59
7	solvent disposal	1.80	2.14	[€/kg]		Zweckverband für Abfallwirtschaft in Nordwest-Oberfranken	http://www.zaw-coburg.de/problemmuellsammlungen/kleingewerbe/kosten-kleingewerbe.html
8	solvent disposal	1.51	1.80	[€/kg]		Landkreis Cuxhaven	https://www.landkreis-cuxhaven.de/media/custom/1779_5347_1.PDF?1512659814
9	solvent disposal	1.50	1.79	[€/kg]		Stadt Wolfsburg	www.wolfsburg.de/media/wolfsburg/30_abfallgebuehrensatzung.pdf
10	solvent disposal	2.10	2.50	[€/kg]		Zweckverband Abfallwirtschaft ZAW Donau-Wald	https://www.awg.de/media/recyclinghoefe_zentren_allgemein.pdf
ø		1.55	1.84	[€/kg]			
used	hazardous waste disposal	1.55		[€/kg]			

Supplementary Table S5/6: Cost data sources of material and services for the biosurfactants production cost analysis and S-LCA.

	substrate	price net [€]	price gross [€]	unit	year	supplier	source
transport costs							
1	costs per tonne-kilometre	0.02	0.02	[€/m³]	2016	Deutsche Zentrum für Luft- und Raumfahrt e. V.	https://elib.dlr.de/104581/1/wolfermann-transport_cost_-_an_aggregated_model_for_surface_freight_transport.pdf
2	costs per tonne-kilometre	0.04362	0.05	[€/m³]	2020	Bundesanstalt für Gewässerkunde	https://www.bafg.de/DE/08_Ref/U1/02_Projekte/05_Verkehrstraeger/verkehrstraeger_lang.pdf?__blob=publicationFile
3	costs per tonne-kilometre	0.07084	0.08	[€/m³]	2020	Bundesanstalt für Gewässerkunde	https://www.bafg.de/DE/08_Ref/U1/02_Projekte/05_Verkehrstraeger/verkehrstraeger_lang.pdf?__blob=publicationFile
4	costs per tonne-kilometre	0.4	0.48	[€/m³]	2014	-	Wannenwetsch, H. et al. (2014) Integrierte Materialwirtschaft, Logistik und Beschaffung
5	costs per tonne-kilometre	0.088	0.10	[€/m³]	2012	-	Corsten, H. et al. (2012) Nachhaltigkeit: Unternehmerisches Handeln in globaler Verantwortung
6	costs per tonne-kilometre	0.06	0.07	[€/m³]	2020	Verein Deutscher Zementwerke e.V. (VDZ)	https://www.vdz-online.de/fileadmin/gruppen/vdz/3LiteraturRecherche/Studien/Nachhaltige_Transport_und_Logistikketten_Zementindustrie.pdf
7	costs per tonne-kilometre	0.06	0.07	[€/m³]	2018	Universität Linz	http://www.energieinstitut-linz.at/v2/wp-content/uploads/2018/01/publizierbarer-Endbericht_850079_SeasonalGridStorage_final.pdf
8	costs per tonne-kilometre	0.1	0.12	[€/m³]	2018	Universität Linz	http://www.energieinstitut-linz.at/v2/wp-content/uploads/2018/01/publizierbarer-Endbericht_850079_SeasonalGridStorage_final.pdf
Ø		0.105	0.13	[€/m³]			
used	waste water disposal	0.105		[€/m³]			

Comparison market prices



Supplementary Figure S4: Specific prices of diverse rhamnolipids with different properties purchased by different suppliers from various countries; shown prices are partly extrapolated from €/mg to €/kg, for instance. Chart legend shows surfactant description | producer/seller.

Supplementary Table S6: Specific prices for sophorolipids sorted by price under consideration of purity and packaging size; reflecting a similar tendency of pricing structure like for rhamnolipids

product description	**purity** **[%$_{SL}$]**	**packaging size**	**price** **[€/kg]**	**source**
Sophorolipid 50 %	50	kg range	0.90	https://www.alibaba.com/product-detail/Sophorolipid_60655401914.html?spm=a2700.7724838.2017115.22.127a691b01r1wX
Sophorlipid 100 %	50	kg range	0.90	https://german.alibaba.com/product-detail/sophorolipid-60655401914.html?spm=a2700.7724838.2017115.1.5dae691bSNWtng
Sophorolipid 99 %	99	kg range	0.90	https://www.alibaba.com/product-detail/Sophorolipid_60628100337.html?spm=a2700.7724838.2017115.150.127a691b01r1wX
Sophorolipid 50 %	50	Mg range	6.75	
Biosurfactant Sophorolipid	50	kg range	9.45	https://qilubiogroup.en.alibaba.com/product/60707991909-804398105/Biosurfactants_Sophorolipid.html?spm=a2700.icbuShop.41413.8.709f6a77KW7HhM
Sophorolipid used for agricultural chemicals	50	kg range	10.35	https://www.alibaba.com/product-detail/Sophorolipid-used-for-agricultural-chemicals_60776970081.html?spm=a2700.7724838.2017115.63.10f01e83Kzs9wz
Sophorolipids biosurfactant SL50	50	Mg range	15.92	www.envgreen.cn/offer/582858934819.html?spm=a2615.2177701.autotrace-offerGeneral.1.493a46d3RsgnL7
Factory support Lactonic Sophorolipid	99	kg range	21.6	https://www.alibaba.com/product-detail/Factory-support-Lactonic-Sophorolipid-CAS-148409_60814445984.html?spm=a2700.7724838.2017115.103.10f01e83Kzs9wz
Sophorolipids Biosurfactant SL50	50	kg range	22.5	https://www.alibaba.com/product-detail/Sophorolipids-Biosurfactant-SL50_60740541974.html?spm=a2700.7724838.2017115.72.10f01e83Kzs9wz
Lactonic Sophorolipid/Sophorolipid	99	kg range	25.50	https://german.alibaba.com/product-detail/Factory-Supply-Lactonic-Sophorolipid-Sophorolipid-CAS-60827522768.html?spm=a2700.7724838.2017115.27.5dae691bSNWtng
Biosurfactant Sophorolipid	85	kg range	31.50	https://qilubiogroup.en.alibaba.com/product/60782545006-804398105/Biosurfactant_Sophorolipid_better_than_rhamnolipid.html?spm=a2700.icbuShop.41413.6.709f6a77KW7HhM
Biosurfactant Sophorolipid 99 %	99	kg range	36.00	https://www.alibaba.com/product-detail/High-efficient-Biosurfactant-Sophorolipids-use-for_60773849267.html?spm=a2700.7724838.2017115.246.127a691b01r1wX
Sophorolipid 50 %	50	kg range	54.00	https://german.alibaba.com/product-detail/High-Quality-Raw-Material-Sophorolipid-60251213862.html?spm=a2700.7724838.2017115.9.5dae691bSNWtng
Lactonic Sophorolipid 99 %	99	kg range	79.65	https://www.lookchem.com/product_lower-Price-Lactonic-Sophorolipid/18049075.html
Biosurfactant Sophorolipid 100 %	100	kg range	180.00	
Sophorolipid Food Grade 98%	98	kg range	225.00	https://german.alibaba.com/product-detail/Food-Grade-98-Purity-Sophorolipid-CAS-60628100337.html?spm=a2700.7724838.2017115.147.5dae691bSNWtng
Sophorolipids biosurfactant S40	40	kg range	1,528.20	http://www.envgreen.cn/offer/582533456261.html?spm=a2615.2177701.autotrace-offerGeneral.7.493a46d3RsgnL7
Lactonic (di-acetylated) Sophorolipids	85	g range	57,100.00	https://www.carbosynth.com/carbosynth/website.nsf/(w-productdisplay)/71834A54140D866880257EEC0037FF96
Acidic Sophorolipids mix-acetylated - mixture of $C_{30}H_{54}O_{13}$, $C_{32}H_{56}O_{14}$ and $C_{34}H_{58}O_{16}$	95	g range	57,100.00	https://www.carbosynth.com/carbosynth/website.nsf/(w-productdisplay)/E63A39A62A23BFB480257EEC0038B9C4
Acidic Sophorolipids non-acetylated	95	g range	65,350.00	https://www.carbosynth.com/carbosynth/website.nsf/(w-productdisplay)/CF8CE58F959C2C6780257EEC0038243F
Bola Sophorolipids	95	g range	86,650.00	https://www.carbosynth.com/carbosynth/website.nsf/(w-productdisplay)/2EA4B18429192AA280257DD3003F6913

II. Supplementary chapter S-LCA

Background S-LCA

Relevant social impact categories in the context of surfactant production were identified by the sustainability reports of four German surfactant-producing chemical companies, which show similar focus areas of assessment.[1-4] Criteria of fair salaries, gender equity, accident prevention and trade union aspects can be found in these reports and show their relevance for surfactant production. The applied indicator selection can be underpinned by the following studies and conditions. Although the geographical relation of the present study (Europe) can be called a “socially related safe ground”, which offers one of the highest levels of social protection,[5] the social dimension of sustainability requires a closer examination. Despite the general status, the EU has to deal with different problems associated to social indicators. As stated in the annual report of the European Social Protection Committee,[6] the EU faces some problems regarding social aspects like at-risk-of-poverty rates or inequalities in access to healthcare and in health outcomes. Moreover, the EU member states have not reached the defined aim of “lifting 20 million people out of the risk of poverty or social exclusion” until 2020, for example.[6, 7] Although the evaluation at EU level is a very superordinate and broad reflection, it is worth to look at the national level. The review of German data for salary-related issues shows that the number of employees paid according to (or in line with) collective agreements has decreased over the last 20 years from 80% to 63% and that the share of low wage workers is one of the largest within the European Union (> 22%).[8, 9] Furthermore, the decreased level of organization by workers’ union (from > 30% in the early 90’s to < 20% in the last years) gives reason enough to study the aspect of workers’ rights more closely.[10] The non-adjusted gender pay gap (general difference of wage between women and men) in Germany was still at 21% in 2019, the adjusted pay gap (difference at exactly identical work) was at 6% in 2016,[11] which gives reason to be studied. In relation to health, statistics reveal that compared to most other EU countries, the specific incidence rate per 100,000 persons employed (non-fatal accidents) is clearly higher in Germany and the number of accidents at work by economic activity are clearly higher in the manufacturing sector than in the energy supply sector for example.[12] A closer look at these aspects could help to minimize impacts in these areas by process design. To discuss these aspects further, in this study the method of social LCA (S-LCA) was applied.

Study framework S-LCA

Similar to the goals of the LCA and CA, the goal of the S-LCA was to determine the most relevant social impacts associated with the process chains and an identification of the most contributing processes. The S-LCA focuses on specific social aspects that are affected by certain parts of the process chains. The system boundaries for S-LCA comprise the processing stages as stated for LCA for a biosurfactant production of 15,000 kg per year. With regard to the CMC-based function of the considered process chains, the functional unit "mass of product necessary to fulfill the same specific cleaning performance (SCP) as 1 kg of MEL" was also applied for S-LCA.

Impact categories and indicators S-LCA

The S-LCA guidelines [13] distinguish different stakeholder groups: workers, the local community in which the workplace is situated, the society in which the local community is nested, the heterogeneous group of value chain actors (this can be industry, site owners, banks, governments, etc.), consumers, and with the latest updated guideline version also children. For the production of biosurfactants, this assessment focused on the stakeholder group of workers with the social impacts of fair salary, trade unionism, gender wage gap, and non-fatal accidents at work. The choice of impacts was based on sustainability reports of businesses in the chemical industry (see [1-4]) by identifying relevant social issues in this branch. In the present study, the evaluation of these impact categories is limited to the process chain related background of material and energy flows (see statement in section "Contributing economic sectors"). By using the previously described S-LCA approach and the PSILCA database, results are given in medium risk hours (mrh); whereby a lower impact value can be categorized as the more advantageous result. Information on the used unit, further methodological explanations and the database PSILCA can be found in different publications.[14-16] The results were eventually transferred to SCP-related values to gain a more adequate comparability of RL and MEL.

Applied data for S-LCA

To conduct the S-LCA, all energy and material flows, which enter and leave the system (e.g., molasses, electricity, water, waste), needed to be converted to a single monetary unit. For this, quantity data from LCA and CA was converted to specific monetary input values in US $ per mass of product to define a demand vector for the input-output model (exchange rate: 1.0 € = 1.1 $)[17]. The sectoral structure is given by the database PSILCA, which in turn is oriented to the classification of economic activities by NACE code.[15, 18] The monetary input data of the S-LCA per process stage and economic sector (e.g., specific cost for electricity supply, substrates, etc.), is illustrated in Supplementary Table S7. An extended description of the data processing and methodological desccriptions can be found in Springer et al.[16]

Supplementary Table S7: Input data of the considered process chains for RL and MEL production with substrate molasses (RL_MOL, MEL_MOL) including quantitative data for the invested US $ per kg of product related to economic sector (sectoral demand) and process stage for S-LCA.

product					RL_MOL					
process stage	RL01	RL02	RL03	RL04	RL05	RL06	RL07	RL08	RL09	*total p.e.s.*
unit	$/kg	$/kg	$/kg	$/kg	$/kg	$/kg	$/kg	$/kg	$/kg	$/kg
Agriculture and hunting	376.40	-	-	-	-	-	-	-	-	*376.40*
Electricity and district heat	185.01	0.08	6.86	0.01	1.36	0.12	0.02	0.00	0.03	*193.50*
Gas supply	-	-	0.03	0.00	-	1.29	-	0.01	0	*1.33*
Machines	31.46	-	-	-	-	-	-	-	-	*31.46*
Manufacture of chemical products	-	-	66.33	0.00	96.09	-	41.61	-	-	*204.03*
Manufacture of fabricated metal products	-	8.8	61.37	1.93	6.8	1.13	3.3	1.01	1.21	*85.55*
Manufacture of food products	4.60	-	-	-	-	-	-	-	-	*4.60*
Manufacture of Non-metallic mineral products	-	0.03	0.42	-	1.08	1.38	0.00	0.00	0.00	*2.92*
Manufacture of plastic products	-	-	34.83	-	-	-	-	-	-	*34.83*
Road and pipeline transport	59.66	-	-	-	-	-	-	-	-	*59.66*
Waste disposal and sewerage services	-	-	5.08	-	0.76	21.58	1.16	0.09	-	*28.67*
Water supply	0.00	-	0.33	0.00	-	-	0.00	-	-	*0.33*
total per process stage	*657.13*	*8.91*	*175.25*	*1.95*	*106.1*	*25.50*	*46.09*	*1.11*	*1.24*	***1023.28***

product					MEL_MOL				
process stage	MEL01	MEL02	MEL03	MEL04	MEL05	MEL06	MEL07	MEL08	*total p.e.s.*
unit	$/kg	$/kg	$/kg	$/kg	$/kg	$/kg	$/kg	$/kg	$/kg
Agriculture and hunting	67.94	-	-	-	-	-	-	-	*67.94*
Electricity and district heat	33.39	0.01	1.49	0.00	0.1	0.02	0.02	0.06	*35.09*
Gas supply	-	-	0.00	0.00	0.08	0.01	0.01	0.01	*0.11*
Machines	5.68	-	-	-	-	-	-	-	*5.68*
Manufacture of chemical products	-	-	32.55	0.05	12.7	2.61	2.61	-	*50.51*
Manufacture of fabricated metal products	-	1.72	13.68	0.64	2.84	2.7	1.52	1.14	*24.24*
Manufacture of food products	0.83	-	-	-		-	-		*0.83*
Manufacture of non-metallic mineral products	-	0.00	0.03	-	0.03	0.01	0.01	0.02	*0.10*
Manufacture of plastic products	-	-	6.64	-	-	-	-	-	*6.64*
Road and pipeline transport	10.77	-	-	-	-	-	-	-	*10.77*
Waste disposal and sewerage services	-	-	0.95	-	1.82	0.22	0.22	0.03	*3.24*
Water supply	0.00	-	0.06	0.00	-	0.02	-	-	*0.08*
total per process stage	*118.61*	*1.74*	*55.40*	*0.69*	*17.55*	*5.59*	*4.39*	*1.26*	***205.23***

RL01 sugar beet production and processing; RL02 storage and preparation; RL03 fermentation; RL04 seed fermentation; RL05 precipitation; RL06 precipitation recovery; RL07 extraction; RL08 extraction recovery; RL09 final conditioning and storage; MEL01 sugar beet production and processing; MEL02 storage and preparation; MEL03 fermentation; MEL04 seed fermentation; MEL05 extraction 01 (incl. recovery); MEL06 extraction 02 (incl. recovery); MEL07 extraction 03 (incl. recovery); MEL08 final conditioning and storage; p.e.s. = per economic sector

Results of S-LCA

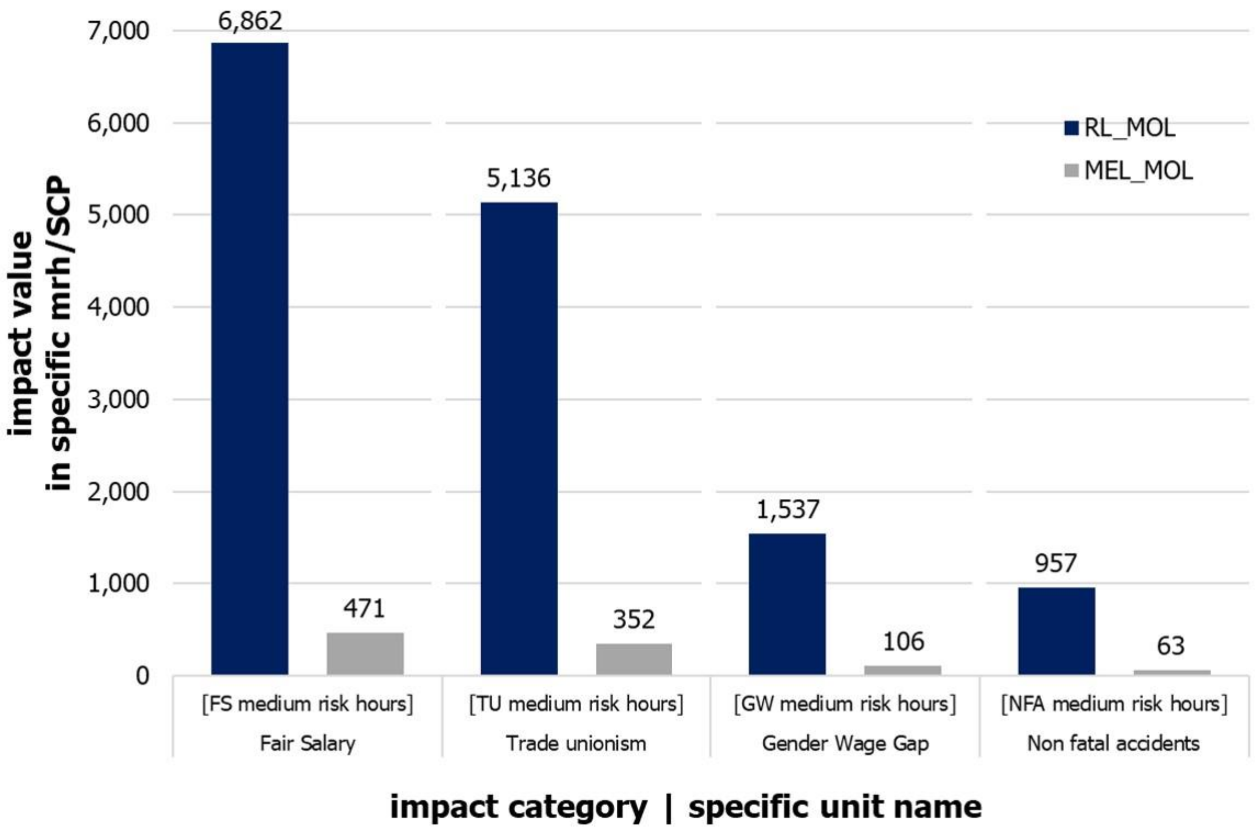
Social Life Cycle Assessment

For S-LCA, the production of RL and MEL only with molasses as a substrate was compared due to the expectation of more significant differences between different products than between different substrates. The following two sections provide results for selected social impacts and contributing economic sectors.

Selected social impacts

The S-LCA reveals impact values of underlying material and energy flows in RL and MEL production. As stated above, these impact values are expressed in medium risk hours (mrh) for each impact category. It is important to note that each impact category has its specific mrh measure, i.e., the impact category fair salary (FS mrh), for instance, cannot be compared with trade unionism (TU mrh) or gender wage gap (GWP mrh). Hence, it is the two types of products that can be compared in specific mrh within one impact category. Supplementary Figure S5 shows that RL production yields roughly 15 times higher mrhs than MEL production, implying higher impacts of detrimental procedures in all considered categories.

This means that the supply chain of RL production bears a considerably higher impact in the assessed impact categories compared to the MEL production. As the results show, it is to be expected that further categories would result in similar ratios of mrhs between RL and MEL production with molasses as a substrate. The same applies for the assessment of SBP as a substrate, due to the given inputs described in section “Applied data”. For further studies it would be useful to include alternative substrates as well as different geographical references (e.g., manufacturing of chemical products in alternative countries) to find the lowest impact level for the production of RL and MEL. Furthermore, the impacts generated by the surfactant production itself, which requires the acquisition of own process-specific data, should be considered in further work.



Supplementary Figure S5: Results for the comparison of RL and MEL production by selected categories of S-LCA per specific cleaning performance (SCP).

Contributing economic sectors

The superiority of MEL over RL regarding social issues raises the question of the responsible economic activities in the respective supply chains. Clearly, the production of RL and MEL differ, entailing different labor intensity in various sectors. In order to reveal these differences, the above-regarded impact categories were additionally examined for the responsible economic sectors (classification by NACE code).[18] For the most relevant sectors, Supplementary Figure S6 gives an overview for each impact category, each graph comparing RL and MEL production. The results reveal that especially the sector “manufacture of chemical products” is the greatest impact driver in all impact categories. “Manufacture of fabricated metal products and of plastic products” also inherit considerable – but smaller – impacts in this supply chain. Obviously, high impact values in chemical, metal, and plastic product manufacturing stem from the combination of the specific indicators’ impact factors (as compiled in internationally recognized databases) and the inventory result, i.e., how much work needs to be done in the specific sectors. As the manufacture of chemical products stands out very clearly in Supplementary Figure S6, a detailed analysis of the required chemical products in both product chains was done. It reveals that in RL production, the need for acetone as a precipitation agent makes up 55% of chemical products (among extraction agent, mineral medium, compressed air, and acidification agent in descending order). This is the case albeit the calculation respects an acetone-recycling rate of 80%. Hence, this agent is an influential driver of social impacts, which should be reduced by means of a higher recycling rate. For MEL production, the use of the mineral medium makes up 64% of chemical products (among extraction agent, compressed air, and acidification agent in descending order). Here, recycling is not possible, as it is consumed by the microorganisms. Hence, it is recommended to evaluate alternative options to limit the social impact of the chemical sector as the greatest driver of social impacts in RL and MEL production.

As mentioned before, the present study does not include impacts associated with the actual operation of the examined production plant. Reasons for the non-availability of data can be seen in the difficulties and high efforts to collect own data for a consideration of labor and the objectives within the related project. Summarized, it is obvious that specific supply chains are mainly responsible for social impacts. The identified impact sources may be influenceable by an adjusted process design and improvements in the field of resource consumption. As an indirect option of reducing the amount of needed chemicals and the coupled social impact, the increase of yields is applicable also in this case, for example.

Supplementary Figure S6: Exemplary results of the S-LCA for the RL and MEL production by selected categories “fair salary” (FS), “gender wage gap” (GW), “Non-fatal accidents” (NFA), and “trade unionism” (TU) per chain specific process/sector.

Literature

1. BASF, *BASF-Bericht 2019 - Ökonomische, ökologische und gesellschaftliche Leistung*, BASF SE, Ludwigshafen, 2020.
2. Bayer, *Nachhaltigkeitsbericht 2019*, Bayer AG, Leverkusen, 2020.
3. Evonik, *Nachhaltigkeitsbericht 2019 - Leading Beyond Chemistry*, Evonik Industries AG, Essen, 2020.
4. Henkel, *Nachhaltigkeitsbericht 2019*, Henkel AG & Co. KG a A, Düsseldorf, 2020.
5. European Parliament, *Social Europe: what Parliament is doing on social policy*, Report REF: 20170616STO77648, European Parliament, 2019.
6. EU-SPC, *Review of the social situation and the development in the social protection policies in the Member States and the Union - 2019 Annual Report from the Social Protection Committee*, EU - Commission Directorate-General for Employement, Social Affairs and Inclusion, Brusseles (BE), 2019.
7. EU-SPC, *2021 SPC annual review of the social protection performance monitor (SPPM) and developments in social protection policies : report on key social challenges and key messages*, Report 9978-92-76-43539-6, Social Protection Committee (SPC), Luxembourg (LUX), 2021.
8. H. Schneider and S. Vogel, *Tarifbindung der Beschäftigten in Deutschland: Eine Auswertung des Sozioökonomischen Panels*, 2018.
9. M. M. Grabka and C. Schröder, *DIW-Wochenbericht*, 2019, 86, 249-257.
10. A. Hassel and W. Schroeder, *GEWERKSCHAFTEN 2030 - Rekrutierungsdefizite, Repräsentationslücken und neue Strategien der Mitgliederpolitik*, Wirtschafts- und Sozialwissenschaftliches Institut (WSI) der Hans-Böckler-Stiftung, Düsseldorf, 2018.
11. BMFSFJ, *Report by the Federal Govern-ment on the effectiveness of the Act to Promote Transparency in Wage Structures among Women and Men*, The Federal Ministry for Family Affairs, Senior Citizens, Women and Youth (BMFSFJ), 2020.
12. Eurostat, *Accidents at work statistics*, https://ec.europa.eu/eurostat/statistics-explained/index.php?title=Accidents_at_work_statistics, accessed 01.03.2023).
13. UNEP, *Guidelines for Social Life Cycle Assessment of Products and Organizations 2020,* United Nations Environment Programme (UNEP) / Life Cycle Initiative / Social LC Alliance, Nairobi (KEN), 2020.
14. C. Di Noi, A. Ciroth, L. Mancini, U. Eynard, D. Pennington and G. A. Blengini, *Can S-LCA methodology support responsible sourcing of raw materials in EU policy context?,* The International Journal of Life Cycle Assessment, 2020, **25**, 332-349. DOI: 10.1007/s11367-019-01678-8
15. PSILCA-DB, *PSILCA - Understanding social impacts*. Berlin: GreenDelta GmbH. 2021, https://psilca.net/, (accessed 01.03.2023).
16. S. K. Springer, C. Wulf and P. Zapp, *Potential Social Impacts regarding working conditions of Fuel Cell Electric Vehicles*, International Journal of Hydrogen Energy, 2023, DOI: 10.1016/j.ijhydene.2023.04.034.
17. ECB, Euro foreign exchange reference rates, https://www.ecb.europa.eu/stats/policy_and_exchange_rates/euro_reference_exchange_rates/html/index.en.html, (accessed 01.03.2023).
18. EU, *Regulation (…) Establishing the Statistical Classification of Economic Activities Nace Revision 2 and Amending Council Regulation (Eec) No 3037/90 as Well as Certain Ec Regulations on Specific Statistical Domains.* 2006. https://eur-lex.europa.eu/legal-content/EN/TXT/HTML/?uri=CELEX:32006R1893&from=EN (accessed 01.03.2023