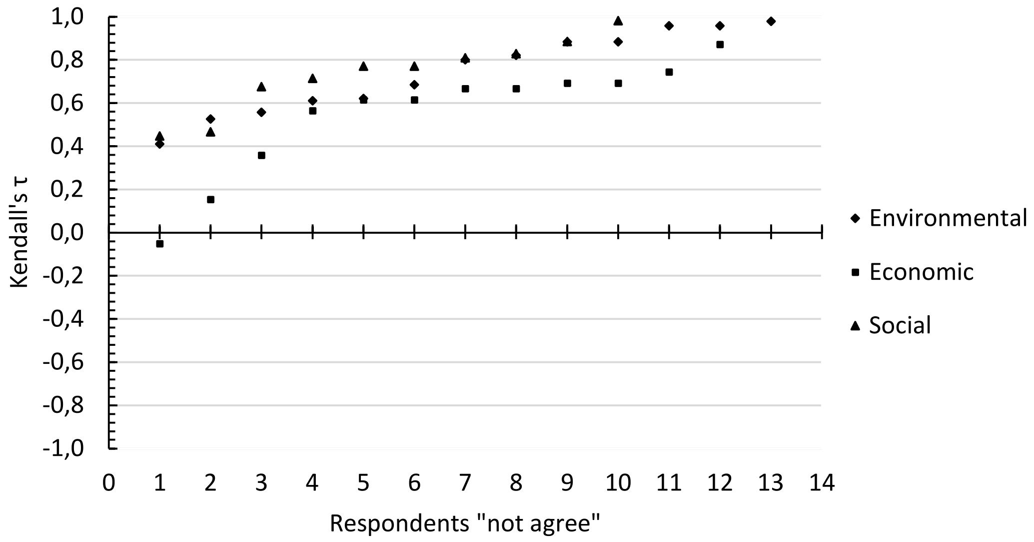
Electronic supplementary information

An integrated techno-sustainability assessment (TSA) framework for emerging technologies

Sophie Van Schoubroeck*, Gwenny Thomassen, Steven Van Passel, Robert Malina, Johan Springael, Sebastien Lizin, Richard A. Venditti, Yuan Yao, and Miet Van Dael.

* Corresponding author: sophie.vanschoubroeck@uantwerpen.be

S.1 Rank correlation coefficient between initial and new rankings.



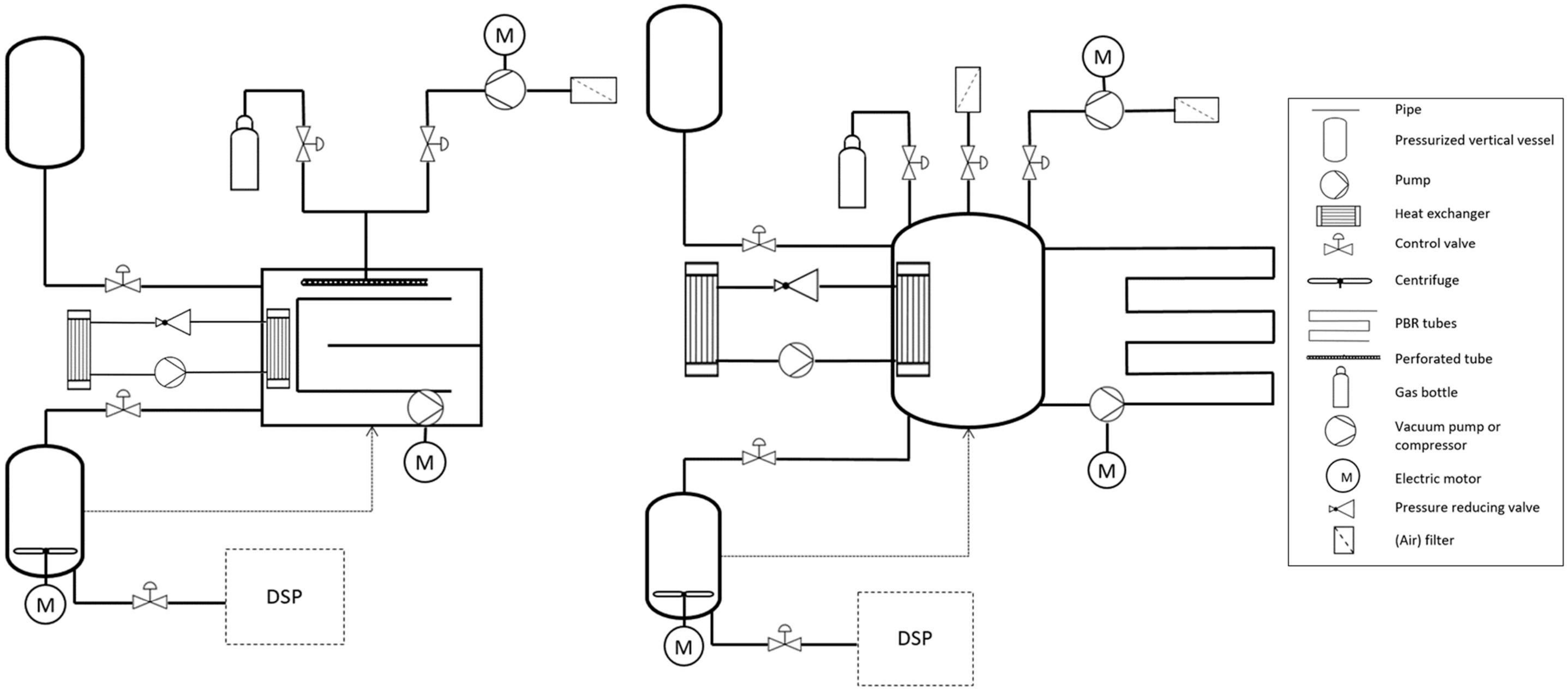
S.2 Kendall’s τ and corresponding z-values.

#respondent	Environmental		Economic		Social	
	τ	z	τ	z	τ	z
1	0.884	5.451	0.692	3.294	0.981	5.097
2	0.958	5.905	0.667	3.172	0.886	4.602
3	0.958	5.905	0.615	2.928	0.829	4.305
4	0.821	5.061	0.615	2.928	0.448	2.326
5	0.411	2.531	0.154	0.732	0.810	4.206
6	0.684	4.218	0.667	3.172	0.714	3.712
7	0.526	3.244	0.744	3.539	0.676	3.514
8	0.611	3.764	-0.051	-0.244	0.771	4.008
9	0.558	3.439	0.564	2.684	0.467	2.425
10	0.884	5.451	0.872	4.149	0.771	4.008
11	0.979	6.035	0.692	4.759	1.000	5.196
12	0.800	4.932	0.359	4.759	1.000	5.196
13	0.621	3.828	1.000	4.759	1.000	5.196
14	1.000	6.164	1.000	4.759	1.000	5.196
15	1.000	6.164	1.000	4.759	1.000	5.196
16	1.000	6.164	1.000	4.759	1.000	5.196
17	1.000	6.164	1.000	4.759	1.000	5.196
18	1.000	6.164	1.000	4.759	1.000	5.196
19	1.000	6.164	1.000	4.759	1.000	5.196
20	1.000	6.164	1.000	4.759	1.000	5.196
21	1.000	6.164	1.000	4.759	1.000	5.196
22	1.000	6.164	1.000	4.759	1.000	5.196
23	1.000	6.164	1.000	4.759	1.000	5.196
24	1.000	6.164	1.000	4.759	1.000	5.196
25	1.000	6.164	1.000	4.759	1.000	5.196
26	1.000	6.164			1.000	5.196

S.3 A frequency analysis of the indicators included (incl.) and excluded (excl.) for a sustainability analysis of algae-based chemicals, based on expert opinion.
Note: the indicators above the dashed line are included in the assessment.

Environmental (n = 26)			Economic (n = 25)			Social (n = 26)		
Indicator	Excl.	Incl.	Indicator	Excl.	Incl.	Indicator	Excl.	Incl.
GHG emissions	1	25	Market potential	0	25	Acceptance of biobased materials	0	26
Raw material efficiency	1	25	Raw materials cost	1	24	Product transparency	0	26
End of life options	2	24	Product innovation	3	22	Job creation	1	25
Ecotoxicity	3	23	Process innovation	4	21	Human toxicity	1	25
Waste generation	1	25	Technical risks	5	20	Income levels	5	21
Energy efficiency	1	25	Capital productivity	6	19	Workplace accidents and illnesses	9	17
Natural land transformation	5	21	Energy cost	6	19	Education and training	7	19
Abiotic fossil depletion	4	22	Land productivity	9	16	Community support and involvement	13	13
Eutrophication	3	23	Product efficiency	10	15	Fatal work injuries	19	7
Agricultural land occupation	4	22	Labor productivity	15	10	Security measures	20	6
Water consumption	3	23	Subsidies	18	7	Social security	21	5
Organic carbon depletion	13	13	Waste disposal cost	16	9	Child labor	18	8
Management practices in crop production	17	9	Transportation cost	20	5	Working hours	23	3
Soil erosion	18	8				Discrimination	22	4
Acidification	22	4				Cultural heritage	22	4
Particular matter formation	23	3						
Abiotic mineral depletion	22	4						
Stratospheric ozone depletion	25	1						
Photo-oxidant formation	26	0						
Ionizing radiation	26	0						

S.4 Technological configuration of different cultivation systems – open pond (left) versus photobioreactor (right). DSP – downstream processing.



S.5 Data inventory.

Note: input numbers can deviate from sources because of unit conversions and additional calculations.

S.5.1 Technological input data TSA.

Cultivation					
Algae specific					
	Porphyridium	**Unit**	**PBR**	**OP**	**Source(s)**
Mass	HNO_3 consumption	g.g biomass^{-1}	0.090	0.090	Supplier information (2019)
	$MgSO_4$ consumption	g.g biomass^{-1}	0.862	1.989	Supplier information (2019)
	Fe DTPA consumption	g.g biomass^{-1}	0.003	0.006	Supplier information (2019)
	H_3PO_4 consumption	g.g biomass^{-1}	0.012	0.012	Supplier information (2019)
	KOH consumption	g.g biomass^{-1}	0.248	0.248	Supplier information (2019)
	CO_2 fixation efficiency	% CO_2	75	41.23	[1–3]
	CO_2 fixation	g.g biomass^{-1}	1.8	1.8	[4]
	Salt use	g.L^{-1}	15	15	Supplier information (2019)
	Phycoerythrin	%	2.18	2.18	[5–8]
Process	Cultivation time	days	10	13	[6,9]
	Growth rate	g.L^{-1}.day^{-1}	0.246	0.082	Averages[10,11]
	Growth photobioreactor (PBR)/ open pond (OP)		3	3	[12]
	Cultivation temperature	°C	20	20	[5,13]
	Water recycling	%	90	90	Assumption
	Salt recycling	%	90	90	Assumption
	Dunaliella salina	**Unit**	**PBR**	**OP**	**Source(s)**
Mass	$MgSO_4$ consumption	g.g biomass^{-1}	0.140	0.775	[14]
	KNO_3 consumption	g.g biomass^{-1}	0.286	1.628	[14]
	$NaHCO_3$ consumption	g.g biomass^{-1}	0.095	0.541	[15]
	KH_2PO_4 consumption	g.g biomass^{-1}	0.008	0.044	[14]
	$FeCl_3.6H_2O$ consumption	g.g biomass^{-1}	0.002	0.009	[14]
	CO_2 fixation efficiency	% CO_2	75	41.23	[1–3]
	CO_2 fixation	g.g biomass^{-1}	1.8	1.8	[4]
	Salt use	g.L^{-1}	117	117	[14]
	β-carotene	%	5.40	5.40	[15,16]

Process	Cultivation time	days	10	23	[17]
	Growth rate	$g.L^{-1}.day^{-1}$	0.197	0.0135	[16,17]
	Cultivation temperature	°C	25	25	[15]
	Water recycling	%	90	90	Assumption
	Salt recycling	%	90	90	Assumption

<u>Equipment specific</u>	**Parameter**	**Unit**	**PBR**	**OP**	**Source(s)**
Process and equipment	Electricity use air blower	kW	1.1		Supplier information (2019)
	Electricity use pumping (liquid)	kW	0.8		Supplier information (2019)
	Electricity use mixing (blower + paddle wheel)	$kW.m^{-3}$		0.00372	[18]
	Electricity use CO_2 supply unit (CSU)	$kWh.t\ CO_2^{-1}$	0	22.2	[19]
	Electricity use medium preparation system (MPS)	$kW.m^{-3}.h$	0.275	0.275	[1]
	Electricity use artificial light	kW	0.056		Supplier information (2019)
	> Artificial light use	$h.day^{-1}$	3		Supplier information (2019)
	> Lamps/ volume PBR	%	0.024		Supplier information (2019)
	Heat loss	$\%.day^{-1}$	30	100	Assumption
	Additional heating due to solar irradiation	°C	5		[17]
	COP heat exchanger	-	3.25	3.25	AquaCal
	MPS hours	h	6	6	[1]
	Mixing hours	h	24	24	Assumption
	Number of reactors	#	20		Supplier information (2019)
	Inoculum system/ reactor volume	$L.L^{-1}$	0.01	0.01	Supplier information (2019)
	Volume ground area	$L.m^{-2}$	36		Supplier information (2019)
	Height pond	m		0.2	[20]
Emissions	N_2O emissions	$kg\ N_2O.kg\ N^{-1}$	0.0039	0.000024	[21]
	NH_3 emissions	$kg\ NH_3.kg\ N^{-1}$	0.05	0.05	[22]
	O_2 emissions	$g.g\ biomass^{-1}$	1.07	1.07	[23]
	Fugitive emissions open ended line	$kg.h^{-1}$	0.002	0.002	[24]
	Fugitive emissions tank	$kg.h^{-1}$	0.082	0.082	[24]
	Fugitive emissions pumping (liquid)	$kg.h^{-1}$	0.0199	0.0199	[24]

Harvesting	**Parameter**	**Unit**		**Source(s)**
Process and equipment	Biomass loss	%	3	[17]
	Maximum concentration	%DW	12	[25]
	Electricity use centrifuge	$kWh.m^{-3}$	1.4	[26]

	Operating hours	h	24	Assumption
Emissions	Fugitive emissions centrifuge light liquid	$kg.h^{-1}$	0.0199	[24]

Others	Parameter	Unit		Source(s)
	Average temperature Belgium	°C	11.50	KMI (2020)
	Average temperature France	°C	12.77	Tradingeconomics (2020)
	Operation rate	%	90	Assumption

S.5.2 Economic input data TSA.

	Parameter	Unit		Source(s)
General	Evaluation period	yr	10.00	Assumption
	Nominal discount rate	%	15.00	[27]
	Equity - Debt ratio	%	20-80	Assumption
	Interest rate	%	4.50	Assumption
	Inflation rate	%	2.00	Eurostat (2019)
	Tax rate Belgium|France	%	29|33.30	OECD (2019)
	CEPCI October 2019	Index	599.30	[28]
	Site preparation	$\%I_0$	10	[29]
CAPEX	Cost PBR	$€.m^{-3}$	15,571 capacity $[m^3]^{-0.103}$	[1] and supplier information (2019)
	Lifetime PBR	yr	10.00	[1]
	Cost liner	$€.ha^{-1}$	90,438	[30–32]
	Lifetime liner	yr	20	[33]
	Cost paddle wheel	$€.ha^{-1}$	11,776	[30,31,34]
	Lifetime paddle wheel	yr	20	[34]
	Cost inoculum	$€.ha^{-1}$	144,999	[35] and supplier information (2019)
	Lifetime inoculum	yr	20	[32]
	Cost MPS	$€.m^{-3}.h$	7,144 capacity $[m^3.h^{-1}]^{-0.484}$	[1,35]
	Lifetime MPS	yr	10	[35]
	Cost artificial lighting	$€.unit^{-1}$	9	Gamma (2019)
	Lifetime artificial lighting	Yr	10	Gamma (2019)
	Cost heat exchanger	$€.m^{-3}$	702 capacity $[m^3]^{-0.013}$	Supplier information (2019)
	Lifetime heat exchanger	yr	15	[17]
	Cost centrifuge	$€.L^{-1}.h$	6,130 capacity $[L.h^{-1}]^{-0.425}$	Supplier information (2019)
	Lifetime centrifuge	yr	10	[35]

OPEX	Price salt	€.t^{-1}	71	USGS - National Minerals Information Center (2017)
	Purchase price CO_2	€.t^{-1}	80	[36]
	Purchase price HNO_3	€.t^{-1}	707	Alibaba (2019)
	Purchase price $MgSO_4$	€.t^{-1}	297	Alibaba (2019)
	Purchase price FeDTPA	€.t^{-1}	13,559	Mbferts (2019)
	Purchase price H_3PO_4	€.t^{-1}	9,323	Alibaba (2019)
	Purchase price KOH	€.t^{-1}	1,843	Alibaba (2019)
	Purchase price KNO_3	€.t^{-1}	1,594	Mbferts (2019)
	Purchase price $NaHCO_3$	€.t^{-1}	870	Intra Laboratories (2019)
	Purchase price KH_2PO_4	€.t^{-1}	1,993	Mbferts (2019)
	Purchase price $FeCl_3.6H_2O$	€.t^{-1}	488	Alibaba (2019)
	Labor cost	€.h^{-1}	39.70	Eurostat (2019)
	Working hours/day Belgium|France	h.day^{-1}	7.6|7	ILO (2019)
	Working days	days	260	ILO (2019)
	Wage rate personnel Belgium|France	€.h^{-1}	40.5|36.6	Eurostat (2019)
	Personnel on-site	Persons	3	[31]
	Hectare for one additional person	ha.PBR^{-1}	10	[17]
	Hectare for one additional person	ha.OP^{-1}	30	[17]
	Electricity cost Belgium|France	€.MWh^{-1}	138.8|113.6	Eurostat (2019)
	Natural gas cost	€.MWh^{-1}	23.3	Eurostat (2019)
	Insurance cost	%I_0	1	[37]
	Repair cost	%I_0	1	Assumption
	Water purchase cost	€.m^{-3}	3.76	VMM (2020)
	Water disposal cost	€.m^{-3}	2	VMM (2020)
Revenues	Selling price phycoerythrin	€.kg^{-1}	36,000	[38]
	Selling price β-carotene	€.kg^{-1}	1,183	[39]
	Total market size food colorants	t.yr^{-1}	450,000	[40]

S.5.3 Environmental input data TSA.

Characterization factors are retrieved from the Ecoinvent 3.5 database. The additional information needed is found in the tables below.

PBR (/unit)	Unit		Source
Scale: length	m	5,800	Supplier information (2019)
Scale: volume	m³	18	Supplier information (2019)
Scale: sizing factor		0.897	Economic regression
Input: borosilicate glass	kg	5,800	Supplier information (2019)
Input: steel	kg	2,000	Supplier information (2019)
Input: PET	kg	49	Supplier information (2019)
Input: EPDM	kg	98	Supplier information (2019)
Input: PP	kg	70	Supplier information (2019)
Input: PE	kg	100	Supplier information (2019)
Input: RVS (steel)	kg	70	Supplier information (2019)

Liner (/unit)			
Scale: surface	ha	0.81	[34]
Scale: sizing factor		1	Economic regression
Mass: material		HDPE	[32]
Mass: liner thickness	mil	40	[32]
Mass: liner width	m	12.2	[34]
Mass: additional height	m	0.05	[17]
Mass: liner depth	m	0.2	[14]
Mass: HDPE	kg	81,444	Calculated

Paddlewheel (/unit)	Unit		Source
Scale: surface	ha	0.81	[34]
Scale: sizing factor		1	Economic regression
Input: paddle width	m	12.2	[34]
Input: paddle thickness	m	0.01	[17]
Input: paddle radials		8	[30]
Input: paddle material		HDPE	[41]
Input: engine material		steel	[41]
Input: engine steel	kg	83	Rotary power (2019)
Input: paddle depth	m	0.15	[14]
Input: HDPE	kg	141.31	Calculated

Centrifuge (/unit)			
Scale: input flow	$L.h^{-1}$	4,000	Supplier information (2019)
Scale: sizing factor		0.575	Economic regression
Input: steel	kg	2,905	Supplier information (2019)

S.5.4 Additional social input data TSA – a proxy for transparency.

The transparency proxy was calculated for all countries within the EU for which data is available on the OECD website (2017). No data was found for Bulgaria, Croatia, Greece, Ireland, Romania, Slovakia, Malta, and Cyprus. The lowest transparency is present in Slovenia and the highest in Luxembourg and Finland. These numbers are specifically calculated for transparency in the food and chemical sector. The higher the proxy number, the better.

Country	***# companies in manufacturing of chemical products***	***# companies in manufacturing of food products***	***# sustainability reports in food and chemicals***	***Transparency proxy***
Slovenia	218	2,263	0	0
Portugal	843	9,327	1	0.0098
Italy	4,250	52,542	9	0.0158
Poland	2,487	14,436	4	0.0236
France	3,042	51,288	13	0.0239
Spain	3,542	23,151	10	0.0375
Czech Republic	1,793	8,087	4	0.0405
Lithuania	143	1,541	1	0.0594
Latvia	228	1,055	1	0.0779
Belgium	614	6,720	6	0.0818
Germany	3,019	21,498	23	0.0938
Hungary	672	4,558	6	0.1147
Austria	370	3,535	5	0.1280
Estonia	126	640	1	0.1305
Sweden	833	3,868	9	0.1914
United Kingdom	2,897	8,036	22	0.2012
Netherlands	912	5,924	14	0.2048
Denmark	277	1,466	4	0.2295
Finland	290	1,610	12	0.6316
Luxembourg	16	125	1	0.7092

S.6 Indicator quantification.

Environmental

Most environmental indicators selected by the experts in the present study are calculated using the ReCiPe characterization factors and the Ecoinvent 3.5 database (allocation at point of substitution - unit). It is important to note that other LCIA methods, such as the one recommended by the International Reference Life Cycle Data System (ILCD), can be selected by the decision-maker. The ReCiPe characterization factors of global warming potential (GWP) are used to quantify the indicator *GHG emissions* in kg CO_2 equivalents. For the *ecotoxicity* indicator, terrestrial, freshwater, and marine ecotoxicity are calculated expressed in kg 1.4 dichlorobenzene (1.4-DB) equivalents to industrial soil, freshwater, and marine water. The ReCiPe method defines *land use* impact as the category that reflects "the process of land transformation, land occupation, and land relaxation".[42] The ReCiPe method calculates land occupation, transformation, and organic carbon depletion in one land use indicator, expressed in m^2 years crop equivalents. Fossil resource scarcity is quantified to measure the *abiotic fossil depletion*, expressed in kg oil equivalents. *Eutrophication* is measured as freshwater and marine eutrophication from the ReCiPe indicator set, expressed in kg phosphor (P) and kg nitrogen (N) equivalents. Finally, *water consumption* is calculated using the water depletion characterization factors which correspond to the total amount of water used in m^3.

To avoid double-counting, the indicators *raw material efficiency* and *waste generation* are united and quantified by the calculation of the E-factor. The E-factor was developed in the 1980s by Roger A. Sheldon[43]. It divides kg waste by kg product as shown in Equation (1).

$$\mathrm{E-factor\ (EF)} = \frac{\mathrm{m\ input\ [kg] - m\ output\ [kg]}}{\mathrm{m\ output\ [kg]}} \qquad (1)$$

A higher E-factor means more waste and points to a greater negative environmental impact and extra costs for disposing the waste. Different E-factors were calculated in Table S.6.1 differentiating between inputs with or without water (that is, mass of water is included or not), and outputs referring to total biomass production or product content (that is, phycoerythrin or β-carotene). Independent of the calculation method, Scenario 1 always scores best and Scenario 4 worst. Scenarios 2 and 3 change places depending on the calculation with or without water: the OP scenarios score worse when water is encountered as an input. As water consumption is already calculated by a ReCiPe indicator, mass of water could be excluded from the E-factor calculations for the microalgae case study.

Table S.6.1 Yearly average E-factors.

	SC1	SC2	SC3	SC4
E-factor (biomass output, with water)	81	187	146	662
E-factor (biomass output, without water)	3	7	11	46
E-factor (product output, without water)	205	385	223	904
E-factor (product output, with water)	3,888	8,866	2,808	12,660

End-of-life options is described as 'the possibility for recycling, composting, biodegrading, burning, … the end product'.[44] In the present case study, the end product is processed as a food colorant, and the packaging materials used for the concerning food dye carry environmental concerns. The up and downstream impacts of paper, steel, and plastic packaging are reflected in the other environmental indicators and 'end-of-life options' was therefore not staged as a separate indicator in the TSA model. This way, double counting can be avoided. For the microalgae case, the end of life impacts per kg pigment is considered the same for all scenarios. As a consequence, these are not included in a comparative analysis.

The last environmental indicator to quantify is *energy efficiency*. Juodeikiene et al. (2015) quantify energy efficiency by dividing the total energy input by the caloric value (higher heating value) of the end product.[45] However, a determination of the caloric value is especially useful when the end product involves an energy-related output like algae-based biofuels. Within the case, the end products are biobased chemicals, and focus will be placed on the energy consumption per kg of product output, instead of caloric values (Equation (2)).

$$\text{Specific energy consumption (SEC)} \left[\frac{\text{MWh}}{\text{kg}}\right] = \frac{\text{Energy}_{\text{input}}[\text{MWh}]}{\text{Product}_{\text{output}}[\text{kg}]} \qquad (2)$$

Energy consumption provides a first estimation but when moving to a higher TRL towards a full-scale company, the energy efficiencies should be estimated or an exergy analysis could be applied to expose the inefficient processes.[46] For the microalgae case, the energy consumption of Scenario 4 scores three to nine times higher compared to the other scenarios. This could be explained by the low β-carotene output and the need for additional heat, using a heat exchanger to grow the algae.

Economic

At low TRL, the *market potential* can be calculated based on the market size and price of the end product. Scenarios 1 and 2 include the price for phycoerythrin. Scenarios 3 and 4 the price for β-carotene. World usage of food colors was estimated at 40,000 to 50,000 tonnes in 2013.[40] No data is publicly available about the share of different colors within the market. It is assumed that their market share within the natural food color market will be the same. As a consequence, only prices were compared to evaluate the market potential for this case study. Legal factors were disregarded, and an assumption was made that both pigments would be allowed in the European food market in the future. Next to its application as a food colorant, phycoerythrin can be sold as a highly valuable biomolecule in niche markets at 254 €.mg^{-1}.[8] However, the present study aims for a larger product market (i.e. food colorants) and takes into account the price of phycobiliproteins which varies from 2.5 €.mg^{-1} to 21.2 €.mg^{-1}.[38] The price of β-carotene varies from 215 €.kg^{-1} to 2,150 €.kg^{-1}.[39] Both prices for phycoerythrin and β-carotene vary a lot in literature. It was decided to hold a 'low' price of 36,000 €.kg^{-1} for phycoerythrin because prices at the upper range consider applications in health research such as fluorescent probes.[39] For the price of β-carotene, an average of 1,183 €.kg^{-1} was considered in the present study.

Technical risks are defined as risks associated directly with the supply chain activities, e.g. feedstock supply risk, infrastructure risk, etc.[44] Patel et al. (2012) have proposed the Risk Aspects (RA) indicator which can be used to measure the technical risks.[47] They defined sub-indicators that are needed to assess risk: (i) Feedstock supply risk, (ii) regional feedstock availability, (iii) market risk, (iv) infrastructure risk, and (v) application-technical aspects (i.e. inherent functional and pathway aspects). Weights are determined by the CatchBio project based on expert opinion.[47] Table S.6.2 gives an overview of the scores calculated for the four algae scenarios on the different risk aspects. The higher the scores, the higher the risks. These scores are based on literature and market information. Although the end-product is made from algae, it is water, salt, additional nutrients, and CO_2 that are used as feedstock to cultivate the algae. These feedstocks are largely and regionally available, which means a score of 0 is given to all scenarios. Market risk is small as food dyes are existing commodity chemicals. According to the scoreboard described in Patel et al. (2012), this yields a score of 0.33 for every scenario. The infrastructure risk is the criterion that creates a difference between the scenarios. The target product phycoerythrin as a food colorant would need new processing and supply chains while β-carotene is already commercially produced as a food dye. In addition, the cultivation technology changes the infrastructure risk as the technologies used for open ponds are more mature than the technologies for horizontal photobioreactors. For PBR technologies, new processing plants would be required. The application-technical risk aspects are the same for both pigments.

Table S.6.2 Risk Aspects (RA). Higher score = higher risk.

	Weights	SC1	SC2	SC3	SC4
Feedstock supply risk	0.25	0	0	0	0
Regional feedstock availability	0.15	0	0	0	0
Market risk	0.25	0.33	0.33	0.33	0.33
Infrastructure (availability) risk	0.20	0.66	0.66	0.33	0
Application-technical aspects	0.15				
Chemicals: functional groups	0.50	0.50	0.50	0.50	0.50
Chemicals: retention of raw material functionality	0.50	0	0	0	0
Final score		**0.25**	**0.25**	**0.19**	**0.12**

The RA indicator offers a proxy for the technical risks, but it does not take into account every risk aspect. For example, OP technology generally has a higher risk of contamination compared to closed systems and thus, at a large scale, the risk of losing large batches of algae feedstock.[9] Closed photobioreactors have the advantage of better control on culture conditions such as CO_2 supply and temperature control.[48]

Product- and process innovation are two other economic indicators to measure sustainability.[44] Patent analysis has been used to assess product and process innovation.[49–51] Patents can be considered as the outputs from the innovation process.[52] A point of critique is that it rather reflects inventiveness than innovation. Also, some technological advances might not be patentable and companies and research institutes can have other methods of protecting their technological advantage.[52] However, patents have proven to present a close link to economic relevant inventions.[50] At low TRL, the number of patents approved is considered an interesting proxy for product and process innovation within the present study. The more patents published, the higher the degree of innovation. A patent count was performed on Espacenet, a database provided by the European Patent Office. The results of this analysis are presented in Table S.6.3. It is not the aim of the present study to perform a detailed patent analysis, but including additional information such as the average number of scientific citations, geographical origin, and time-scales could improve such analysis in the future.[50] Considering process innovation in the past 10 years, the scenarios including pond cultivation technologies score better compared to photobioreactors. For product innovation, most patents were counted for β-carotene but differences with phycoerythrin are small.

Table S.6.3 Patent count [search July 2020]. # = number of patents; and $\#_{10}$ = number of patents published in 2010-2020.

Search queries [in title, abstract, or claims]					**#**	**Publication range**	**$\#_{10}$**
		AND	AND	AND			
Product	"dye" OR "colorant"	"betacarotene"	"algae"		32	1984-2019	22
				"food"	9	2007-2018	8
		"phycoerythrin"	"algae"		25	1994-2019	16
				"food"	2	2014, 2017	2
Process	"algae"	"cultivation" OR "cultivating"	"pond"		1,634	1973-2020	1,440
			"photobioreactor"		495	1995-2020	431

Capital productivity divides yearly sales by the average capital cost per year. For the PBR scenarios (that is, Scenarios 1 and 3), the CAPEX of the medium preparation system, bioreactor, heat pump, and artificial lights were taken into account. For the open pond scenarios (that is, Scenario 2 and 4), the medium preparation system, heat pump, liner, and paddle wheel were included. The calculations of capital productivity are shown in Table S.6.4. Higher numbers represent higher productivities. Even though the capital costs of the PBR cultivation were significantly higher compared to the OP, the high price of phycoerythrin resulted in higher sales, which increased the capital productivity for Scenarios 1 and 2.

Table S.6.4 Yearly average capital productivity. [a]Depending on lifetime per equipment.

	SC1	SC2	SC3	SC4
Average capital cost (€)[a]	376,932	192,854	380,609	168,249
Sales (€)	22,161,598	41,039,996	1,037,190	549,747
Capital productivity	**58.79**	**212.80**	**3.79**	**3.27**

The final indicators that were quantified within the economic dimension were the *cost of raw materials* and the *energy cost*. The total costs of raw materials and energy per year were divided by the total product output. The cost of raw materials calculation included the cost of salt, water, fertilizers, and CO_2. Both cost indicators should be minimized to achieve more sustainability. Scenario 4 scores the worst on both cost indicators, while Scenario 3 has relatively low costs of raw materials and energy.

Social

Acceptance of biobased materials was selected as the most important social indicator by the microalgae experts in Step 2 of the TSA. Although the perception and associated market uptake of biobased products are recognized to be important, a framework for assessment is lacking.[53] Social acceptance is usually assessed qualitatively using focus groups or questionnaires. In contrast, choice-based experiments to investigate consumers' willingness to pay (WTP) have been used in the past to assess consumer acceptance of food in a quantitative way.[54–56] Within the present study, two different algae-strains were compared for the same output i.e. food dyes. The acceptance of the algae-based food colorants was considered the same in all scenarios as it is assumed that customers will not deviate between algae strains. Customers will not resist using a product based on information of that it is being produced from a specific algae strain. Assessing the acceptance would be more relevant if a synthetic benchmark would be included. Previous research from Bearth et al. (2014) and Gebhardt et al. (2020) assessed consumers' expectance and concluded artificial food dyes are disliked more by the public compared to natural alternatives.[57,58] A synthetic alternative was not assessed and as a consequence, customer acceptance is considered the same for all scenarios assessed in the present study.

Product transparency is usually measured in a qualitative or semi-quantitative way. According to the Social-LCA methodological sheets developed by UNEP and SETAC in 2013, transparency should enable the consumer to make an informed choice without intent to mislead or conceal.[59] They propose two ways of measuring transparency: a specific and generic analysis. When analyzing a technology at low TRL, a specific analysis as proposed by UNEP and SETAC is rather difficult. The specific analysis focuses on indicators such as 'consumer complaints regarding transparency', 'publication of a sustainability report', or 'company rating in sustainability indices', where data should be found on a company's website, by interviews with their customers or management, or from the Dow Jones Sustainability index. The generic analysis proposed by UNEP and SETAC offers two indicators which can be used for technology assessment at a lower TRL: 'presence of a law or norm regarding transparency (by country and/or sector)' and 'sector transparency rating: number of organizations by sector which published a sustainability report'. These two generic indicators rely on country and sector data, which can already be evaluated at low TRL. Data was collected for Belgium and France within the Global Reporting Initiative (GRI) database in the chemistry- and food sector (2017). Other reporting databases might be selected if deemed relevant for the assessed sector. The country-specific GRI data is compared relative to the number of enterprises present. As the indicator considers the effective implementation of sustainability reporting, this proxy for transparency can be chosen as an input for the TSA (Table S.6.5). A higher proxy number leads to a higher level of transparency. It was assumed that the entire value chain is located in Belgium for Scenarios 1 and 2 and in France for Scenarios 3 and 4. When more data become available, more specific assumptions can be made about the location of the different processes along the value chain. To provide a benchmark, the transparency proxy was calculated for all countries within the EU for which data is available on the OECD website (ESI S.5.4). Belgium scores better on the transparency proxy compared to France. However, this difference is rather small compared to other EU countries.

Table S.6.5 Transparency proxy. [a]OECD, 2017; [b]GRI database, 2017.

	Belgium	France
Manufacture of chemicals and chemical products [a]	614	3,042
Manufacture of food products [a]	6,720	51,288
Total # of enterprises	7,334	51,387
# sustainability reports [b]	6	13
% sustainability reports per enterprise	**0.082**	**0.024**

When technology matures and a full-scale company is assessed, another method to measure organizational transparency is proposed by Zakaria et al. (2018). They developed an indicator of transparency in sustainability reporting which measures the relative entropy between the probability distributions of words in the sustainability dictionary and those in a corporate report.[60]

At low TRL, direct *job creation* is calculated by counting the jobs needed within the cultivation and harvesting step. An integration with technical parameters is possible by making the number of employees dependent on the scale of the plant. As only one hectare of production area is assessed, the direct job creation will be the same for all scenarios (i.e. three employees). Supervision and clerical labor can be estimated as 10 to 20 percent of the operating labor.[37] To include indirect job impacts, input-output multipliers can be determined, which represent an additional or direct change to the economy resulting from each change in a selected industry.[61] This is done for an algal biofuel manufacturing site by Madugu in 2015. However, input-output multipliers are very case dependent and thus cannot be transferred for use in the present study.

Human toxicity is calculated by using the ReCiPe characterization factors and the Ecoinvent 3.5 database. The carcinogenic as well as non-carcinogenic human toxicity potential (HTP) are both taken into account. Scenario 4 scores the worst on both HTP indicators while Scenarios 2 and 3 score best.

Income levels and the fairness of these incomes can be assessed by calculating the fair wage potential (FWP).[62,63] Neugebauer et al. (2017) developed the FWP taking into account working time, equal remuneration, and living wage (Equation (3)). The Gini-coefficient can be used as an approximation for the income inequalities factor (IEF). Table S.6.6 presents the calculations for the different microalgae scenarios. It was again assumed that the entire value chain is present in one country, i.e., Belgium or France. Under the assumptions made, the scenarios present in Belgium scored better with a higher fair wage potential compared to the French algae production systems.

$$\mathrm{FWP_n} = \frac{\mathrm{RW_n}}{\mathrm{RWT_n}} * \mathrm{CF_{FW,n}}$$
$$\mathrm{CF_{FW,n}} = \frac{1}{\mathrm{MLW_n}} * \mathrm{CWT_n} * (1 - \mathrm{IEF_n^2}) \qquad (3)$$

(with n – process, RW– real (average) wage, RWT – real working time, CF – fair wage characterization factor, MLW – minimum living wage, CWT – contracted working time, and IEF – inequality factor)

Table S.6.6 Fair wage potential: Belgium versus France. [a]Real (average) wage – OECD 2018; [b]Real working time (RWT) – Eurostat 2018; [c]Min. living wage (MLW) – Eurostat 2018; [d]Contracted working time (CWT) – ILO 2009; [e]Inequality factor (IEF) – Gini 2015.

	RW[a] €/month	RWT[b] hours/week	MLW[c] €/month	CWT[d] hours/week	IEF[e] %	**FWP**
Belgium	3,677.97	41.0	1,330	38	0.277	**1.340**
France	3,143.36	40.4	1,510	35	0.327	**0.817**

Finally, a quantification method needs to be found to assess the *workplace accidents and illnesses*. Kidam and Hurme (2013) analyzed 364 equipment's related accident cases within the chemical industry. Process accidents within an equipment category were calculated relative to the other equipment categories.[64] The biggest difference in equipment within the microalgae case study is the use of an OP versus a PBR which can be categorized as a 'storage tank' and 'reactor' holding the same accident rate. Both 'storage tanks' and 'reactors' are each responsible for 14 percent of the accidents.[64] However, the number of accidents per equipment type is not only dependent on the risks per equipment but also a function of the required labor.[65] In the microalgae case assessed within the present study, required labor was in all cases considered the same. Consequently, workplace accidents will not deviate between the scenarios.

S.7 Sensitivity analysis.

The sensitivity analysis is performed using Oracle Crystal Ball software, 10,000 trials, varying all input data by -10% to +10% following a triangular distribution. The following tables show all Spearman's rho (i.e., a rank correlation coefficient) values, which are ≥ 0.2.

Environmental

Parameter	Unit	GHG	TETP	METP	FETP	LUP	AFD	FEP	MEP	WCP	EF	SEC
SCENARIO 1												
Recycled water	%									-0.8		
Recycled salt	%		-0.23	-0.21	-0.2				-0.24		-0.69	
Growth rate	$g.L^{-1}.day^{-1}$	-0.46	-0.39	-0.47	-0.46	-0.5	-0.49	-0.47	-0.45	-0.32	-0.2	-0.55
CO_2 fixation	$g.g\ biomass^{-1}$		0.24								-0.29	
Pigment content	%	-0.66	-0.72	-0.63	-0.63	-0.55	-0.6	-0.65	-0.62	-0.36	-0.55	-0.57
CO_2 eq.	$impact.kg^{-1}$		0.24									
Artificial light ratio	%	0.2		0.21	0.2	0.26	0.22	0.2	0.21			0.31
Artificial light	$h.day^{-1}$				0.22	0.26	0.24		0.21			0.3
Artificial light power	kW	0.22			0.21	0.26	0.23	0.21	0.21			0.3
Electricity eq.	$impact.kWh^{-1}$	0.36		0.33	0.34	0.43	0.39	0.34	0.34			
SCENARIO 2												
Recycled water	%									-0.45		
Pigment content	%	-0.97	-0.97	-0.97	-0.97	-0.97	-0.95	-0.97	-0.97	-0.84	-0.96	-0.93
SCENARIO 3												
Cultivation time	#days										-0.2	
Recycled salt	%			-0.2				-0.25	-0.21		-0.48	
Growth rate	$g.L^{-1}.day^{-1}$	-0.64	-0.64	-0.67	-0.67	-0.67	-0.66	-0.64	-0.66	-0.7	-0.56	-0.72
Pigment content	%	-0.71	-0.7	-0.65	-0.67	-0.67	0.69	-0.67	-0.66	-0.64	-0.62	-0.64
SCENARIO 4												
Recycled water	%									-0.41		
Recycled salt	%		-0.48	-0.48	-0.5	-0.46		-0.5	-0.54		-0.58	
Growth rate	$g.L^{-1}.day^{-1}$	-0.43	-0.34	-0.41	-0.38	-0.39	-0.44	-0.37	-0.36	-0.41	-0.34	-0.46
Pigment content	%	-0.8	-0.75	-0.74	-0.72	-0.74	-0.77	-0.73	-0.71	-0.74	-0.67	-0.76
Dunaliella optimal temperature	°C	0.26					0.31					0.34

Economic

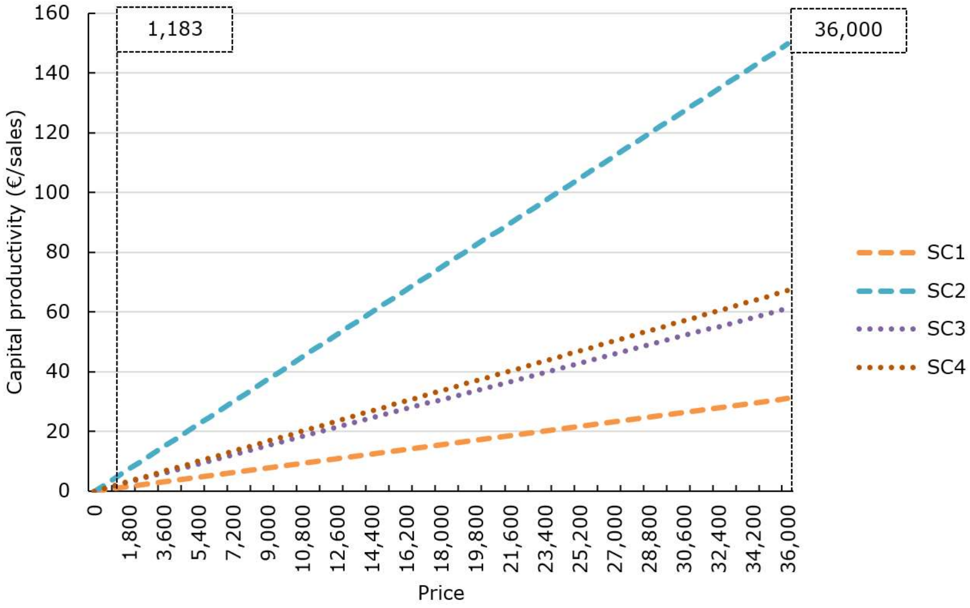
Parameter	Unit	RMC	EC	CP
SCENARIO 1				
Recycled water	%	-0.59		
Cultivation time	#days	-0.21		
Growth rate	$g.L^{-1}.day^{-1}$	-0.23	-0.49	0.49
Pigment content	%	-0.59	-0.5	0.48
Electricity price	$€.MWh^{-1}$		0.48	
Pigment price	$€.kg^{-1}$			0.48
Artificial light ratio	%		0.28	
Artificial light	$h.day^{-1}$		0.29	
Artificial light power	kW		0.28	
PBR cost constant	$€.m^{-3}$			-0.41
PBR cost power	$€.m^{-3}$			-0.25
KOH consumption	g.g $biomass^{-1}$	0.21		
SCENARIO 2				
Pigment content	%	-0.96	-0.93	0.91
CEN cost power	$€.L^{-1}.h^{-1}$			-0.21
SCENARIO 3				
Cultivation time	#days	-0.25		
Recycled salt	%	-0.24		
Growth rate	$g.L^{-1}.day^{-1}$	-0.65	-0.72	0.71
Pigment content	%	-0.63	-0.62	0.62
SCENARIO 4				
Recycled salt	%	-0.3		
Growth rate	$g.L^{-1}.day$	-0.44	-0.45	0.48
Pigment content	%	-0.79	-0.76	0.79
Dunaliella optimal temperature	°C		0.32	

Social

Parameter	Unit	HTP_c	HTP_{nc}
SCENARIO 1			
Recycled salt	%		-0.31
Growth rate	$g.L^{-1}.day^{-1}$	-0.55	-0.44
Pigment content	%	-0.67	-0.66
Electricity eq.	$impact.kWh^{-1}$	0.23	0.29
Steel eq.	$impact.kg^{-1}$	0.22	
SCENARIO 2			
Pigment content	%	-0.97	-0.97
SCENARIO 3			
Recycled salt	%		-0.28
Growth rate	$g.L^{-1}.day^{-1}$	-0.7	-0.65
Pigment content	%	-0.66	-0.65
SCENARIO 4			
Recycled salt	%	-0.44	-0.49
Growth rate	$g.L^{-1}.day^{-1}$	-0.41	-0.39
Pigment content	%	-0.75	-0.73

List of abbreviations: GHG – greenhouse gas emissions, TETP/METP/FETP – terrestrial/marine/freshwater ecotoxicity potential, LUP – land use potential, AFD – abiotic fossil depletion, FEP/MEP – freshwater/marine eutrophication potential, WCP – water consumption potential, EF – E-factor, SEC – specific energy consumption, RMC – raw materials cost, EC – energy cost, CP – capital productivity, MP – market potential, and HTP c/nc – human toxicity potential cancer/non-cancer.

S.8 What-if analysis – the effect of pigment price on capital productivity.



S.9 Indicator values for 43,300 trials – A Monte Carlo simulation.

Note: all the below values are converted to a non-beneficial (minimizing) shape to be compliant with the SMAA models.

SC1	**AFD**	**CP**	**EC**	**EF**	**FEP**	**FETP**	**FWP**	**GHG**	**HTP_C**	**HTP_{NC}**	**LUP**	**MEP**	**METP**	**PCI**	**PDI**	**PT**	**RA**	**RMC**	**SEC**	**TETP**	**WCP**
Base	156	-31	181	205	0.21	17	-1.34	626	27	373	36	0.03	23	-431	-16	-0.08	0.25	63	1.37	1,945	8
Mean	167	-24	194	230	0.22	19	-1.35	672	30	407	39	0.03	25	-474	-17	-0.1	0.25	71	1.48	2,096	10
Min	77	-69	81	108	0.11	9	-1.97	322	14	194	13	0.01	12	-517	-19	-0.12	0.25	34	0.63	1,045	3
Max	491	-5	623	657	0.65	56	-0.91	1,905	90	1,182	146	0.09	75	-431	-16	-0.08	0.25	188	4.71	5,681	32
SC2	**AFD**	**CP**	**EC**	**EF**	**FEP**	**FETP**	**FWP**	**GHG**	**HTP_C**	**HTP_{NC}**	**LUP**	**MEP**	**METP**	**PCI**	**PDI**	**PT**	**RA**	**RMC**	**SEC**	**TETP**	**WCP**
Base	223	-150	51	385	0.13	15	-1.34	831	14	294	9	0.02	10	-1,440	-16	-0.08	0.25	101	1.96	1,711	7
Mean	240	-113	55	407	0.14	16	-1.35	883	15	309	10	0.02	11	-1,584	-17	-0.1	0.25	107	2.13	1,787	8
Min	107	-310	23	212	0.07	8	-1.97	433	8	167	5	0.01	6	-1,728	-19	-0.12	0.25	53	0.88	1,012	4
Max	768	-25	192	1,053	0.35	40	-0.91	2,518	40	753	25	0.05	27	-1,440	-16	-0.08	0.25	296	7.4	3,965	25
SC3	**AFD**	**CP**	**EC**	**EF**	**FEP**	**FETP**	**FWP**	**GHG**	**HTP_C**	**HTP_{NC}**	**LUP**	**MEP**	**METP**	**PCI**	**PDI**	**PT**	**RA**	**RMC**	**SEC**	**TETP**	**WCP**
Base	33	-2	76	187	0.07	9	-0.82	188	12	216	6	0.02	12	-431	-22	-0.02	0.19	29	0.73	1,113	4
Mean	35	-2	81	257	0.09	10	-0.82	216	14	270	7	0.02	15	-474	-24	-0.03	0.19	37	0.78	1,315	5
Min	17	-7	36	50	0.03	4	-1.2	95	6	86	3	0.01	5	-517	-26	-0.04	0.19	11	0.35	523	2
Max	88	0	222	1,050	0.3	35	-0.56	628	45	956	22	0.07	49	-431	-22	-0.02	0.19	134	2.15	4,119	18
SC4	**AFD**	**CP**	**EC**	**EF**	**FEP**	**FETP**	**FWP**	**GHG**	**HTP_C**	**HTP_{NC}**	**LUP**	**MEP**	**METP**	**PCI**	**PDI**	**PT**	**RA**	**RMC**	**SEC**	**TETP**	**WCP**
Base	561	-2	150	904	0.22	23	-0.82	1,759	28	800	14	0.04	34	-1,440	-22	-0.02	0.12	153	7	2,783	12
Mean	599	-2	160	961	0.24	24	-0.82	1,872	29	851	15	0.04	37	-1,584	-24	-0.03	0.12	163	7	2,951	13
Min	283	-7	75	470	0.12	12	-1.2	905	14	414	8	0.02	18	-1,728	-26	-0.04	0.12	78	3	1,502	6
Max	1,533	0	412	2,394	0.59	60	-0.56	4,711	74	2,131	38	0.11	92	-1,440	-22	-0.02	0.12	413	18	7,088	32

List of abbreviations: SC – scenario, AFD – abiotic fossil depletion, CP – capital productivity, EC – energy cost, EF – E-factor, FEP/MEP – freshwater/marine eutrophication potential, FETP/METP/TETP – freshwater/terrestrial/marine ecotoxicity potential, FWP – fair wage potential, GHG – greenhouse gas emissions, HTP c/nc – human toxicity potential cancer/non-cancer, LUP – land use potential, PCI – process innovation, PDI – product innovation, PT – product transparency, RA – risk aspects, RMC – raw materials cost, SEC – specific energy consumption, and WCP – water consumption potential.

S.10 Pseudocode MCDA model.

```
SMAA()
begin
  Initialize_via_user_input();
  Initialize: Result ← ∅; Rank ← ∅;
  foreach Monte Carlo iteration do
    Initialize
        InputArray ← Read_Monte_Carlo_iteration_from_file();
        listINDMatrixs ← ∅;
        listScoreMatrix ← ∅;
        listTScoreMatrix ← ∅;
    foreach indicator do
      Perform_a_pairwise_comparison_between_each_alternative_scenario();
    end
    Calculate_weighting_scheme();
    listSumWFlows ← Calculate_weighted_sum_of_flows();
    Result ← Result ⊎{listSumWFlows};
    Ranking_of_alternative_scenarios ←
     Transform_listSumWFlows_into_ranking();
    Rank ← Rank ⊎ {Ranking_of_alternative_scenarios};
  end
end
```

```
Inititalize_via_user_input()
begin
  Number_of_scenarios;
  Number_of_indicators;
  Beneficial_vs_non_beneficial_character_of_indicators;
  Weighting_scheme;
  Prior_knowledge_or_not;
  if Prior_knowledge = true then
    Initial_ranking ← ∅;
    foreach indicator do
      Initial_ranking ← Initial_ranking ⊎{rank_value};
    end
    if Weighting_scheme = Rank_Exponent_Weighting then
      Lower_limit_of_exponent_range;
      Upper_limit_of_exponent_range;
    end
  end
  Preference_structure;
  if Preference_structure = level_criterion then
    pLevel;
    qLevel;
  else
    if Preference_structure = linear_preference-indifference then
      pArray ←
       Beneficial_vs_non_beneficial_character_of_indicators ∗ stan-
       dard_deviation_of_the_scores_of_the_alternative_scenarios_on_the_indicators
       /Number_of_alternative_scenarios;
      qArray ← pArray/2;
    end
  end
end
```

```
Perform_a_pairwise_comparison_between_each_alternative_scenario()
begin
    Initialize:
        initPairwiseArray ← matrix_of_zeros;
        initScoreArray ← matrix_of_zeros;
        initTScoreArray ← matrix_of_zeros;
    foreach h ∈ {1, ..., Number_of_indicators} do
        listINDMatrixs ← listINDMatrixs ∪ {initPairwiseArray};
        listScoreMatrix ← listScoreMatrix ∪ {initScoreArray};
        listTScoreMatrix ← listTScoreMatrix ∪ {initTScoreArray};
        foreach i ∈ {1, ..., Number_of_scenarios} do
            foreach j ∈ {1, ..., Number_of_scenarios} do
                listINDMatrixs_hij ← InputArray_jh − InputArray_ih;
                if ((Preference_structure = level_criterion) and
                 (Beneficial_vs_non_beneficial_character_of_indicators*listINDMatrixs_hij
                 > Beneficial_vs_non_beneficial_character_of_indicators* pLevel)) or
                 ((Preference_structure = linear_preference-indifference) and
                 (Beneficial_vs_non_beneficial_character_of_indicators*listINDMatrixs_hij
                 > Beneficial_vs_non_beneficial_character_of_indicators* pArray_h)) or
                 ((Preference_structure = true_criterion) and (Benefi-
                 cial_vs_non_beneficial_character_of_indicators*listINDMatrixs_hij > 0))
                 then
                    listScoreMatrix_hij ← 1;
                else if ((Preference_structure = level_criterion) and (Benefi-
                 cial_vs_non_beneficial_character_of_indicators*listINDMatrixs_hij ⩽
                 Beneficial_vs_non_beneficial_character_of_indicators*qLevel)) or
                 ((Preference_structure = linear_preference-indIfference) and (Benefi-
                 cial_vs_non_beneficial_character_of_indicators*listINDMatrixs_hij <
                 Beneficial_vs_non_beneficial_character_of_indicators*qArray_h)) or
                 ((Preference_structure = true_criterion) and (Benefi-
                 cial_vs_non_beneficial_character_of_indicators*listINDMatrixs_hij ⩽ 0))
                 then
                    listScoreMatrix_hij ← 0;
                else if ((Preference_structure = level_criterion) and
                 (Beneficial_vs_non_beneficial_character_of_indicators*
                 listINDMatrixs_hij >
                 Beneficial_vs_non_beneficial_character_of_indicators*qLevel) and (Bene-
                 ficial_vs_non_beneficial_character_of_indicators*listINDMatrixs_hij ⩽
                 Beneficial_vs_non_beneficial_character_of_indicators*pLevel)) then
                    listScoreMatrix_hij ← 1/2;
                else
                    listScoreMatrix_hij ← (listINDMatrixs_hij − qArray_h) / (pArray_h − qArray_h);
                end
            end
        end
        listTScoreMatrix_h ← listScoreMatrix^t_h;
    end
end
```

```
Calculate weighting scheme()
begin
    Initialize: ws ← ∅;
    if Weighting_scheme = equal_weight then
        foreach  i ∈ {1, ..., Number_of_indicators} do
            ws ← ws ∪⃖ { 1 / (Number of indicators) };
        end
    else if Weighting_scheme = stochastic_random_weighting then
        foreach i ∈ {1, ..., Number_of_indicators} do
            ws ← ws ∪⃖ {random ∈ [0, 1]};
        end
        sumws ← Σ_{i=1}^{Number_of_indicators} ws_i;
        ws ← ws / sumws;
    else if Weighting_scheme = rank_order_centroid_weighting then
        Initial_ranking ← ∅;
        foreach  i ∈ {1, ..., Number_of_indicators} do
            Initial_ranking ← Initial_ranking ∪⃖ {i};
        end
        InitRocwList= ∅;
        foreach j ∈ {1, ..., Number_of_indices} do
            total= 0;
            foreach i ∈ {j, ..., Number_of_indicators} do
                total ← total + 1 / Initial_ranking_i;
            end
            w ← total / Number_of_indicators;
            InitRocwList ← InitRocwList ∪⃖ {w};
        end
        foreach i ∈ {1, ..., Number_of_indices} do
            foreach j ∈ {1, ..., Number_of_indices} do
                if Initial_ranking_i = (j + 1) then
                    ws ← ws ∪⃖ {InitRocwList_j};
                end
            end
        end
```

```
    else
        exp ← uniform random in [Lower_limit_of_exponent_range,
          Upper_limit_of_exponent_range];
        ws ← ∅;
        total ← 0;
        foreach i ∈ {1, . . . , Number_of_indicators} do
            total = total + (Number_of_indicators−i)^exp;
        end
        foreach i ∈ {1, . . . , Number_of_indicators} do
            w ← (Number_of_indicators − Initial_ranking_i + 1)^exp;
            ws ← ws ⟵∪ {w};
        end
    end
end
```

```
Calculate_weighted_sum_of_flows()
begin
    Initialize: listSumWFlows ← ∅;
    foreach do
        scenario
    end
    listSumWFlows ← listSumWFlows ⟵∪ {0};
    foreach h ∈ {1, . . . , Number_of_indicators} do
        foreach i ∈ {1, . . . , Number_of_scenarios} do
            sumTScore ← Σ_{j=1}^{Number_of_scenarios} listTScoreMatrix_hij;
            sumScore ← Σ_{j=1}^{Number_of_scenarios} listScoreMatrix_hij;
            listSumWFlows_i ← listSumWFlows_i + (sumTScore −
              sumScore)∗ws_h;
        end
    end
end
```

S.11 A priori indicator ranking.

Environmental	Economic	Social
1. GHG emissions (GHG)	1. Raw materials cost (RMC)	1. Transparency (PT)
2. Waste generation (EF)	2. Process innovation (PCI)	2. Human toxicity (HTP)
3. Ecotoxicity (ETP)	3. Product innovation (PDI)	3. Income levels (FWP)
4. Energy efficiency (SEC)	4. Technical risks (RA)	
5. Land use (LUP)	5. Capital productivity (CP)	
6. Abiotic fossil depletion (AFD)	6. Energy cost (EC)	
7. Eutrophication (EP)		
8. Water consumption (WCP)		

S.12 SMAA results per weighting scheme at level 1 (in %). SC – scenario, SRW – stochastic random weights, ROCW – rank-order centroid weights, and REW – rank exponent weights.

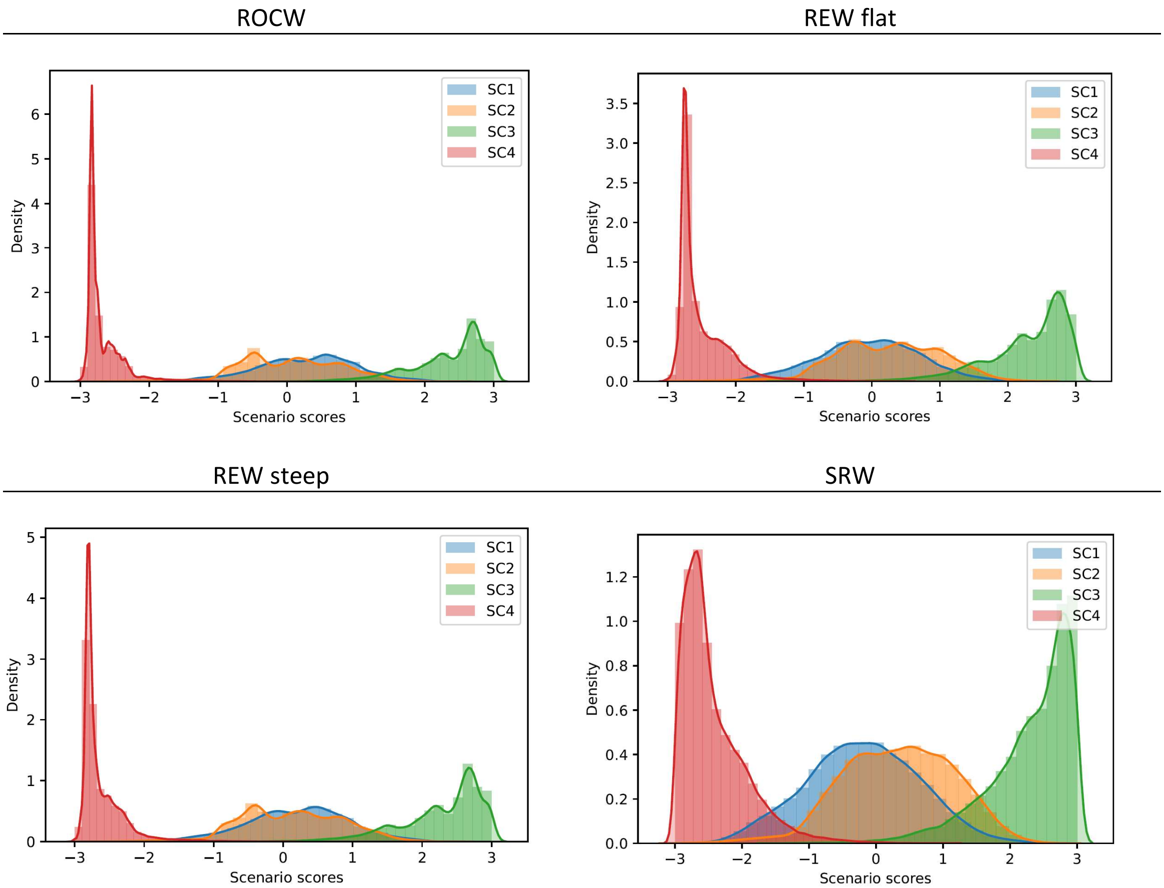
Note: these summarizing ranking results show the percentage of times a certain scenario was ranked at a specific ranking position, with rank 1 being the best alternative with the lowest environmental impact and highest economic and social scores.

		ROCW				**REW flat**				**REW steep**				**SRW**			
		SC1	**SC2**	**SC3**	**SC4**	**SC1**	**SC2**	**SC3**	**SC4**	**SC1**	**SC2**	**SC3**	**SC4**	**SC1**	**SC2**	**SC3**	**SC4**
		Environmental															
Rank position	1	3.64	2.27	94.08	0	2.88	4.45	92.66	0	3.68	3.33	92.99	0	2.64	6.45	90.91	0
	2	53.06	41.82	5.10	0.02	41.65	52.26	5.98	0.12	50.93	43.31	5.75	0.02	34.63	57.39	7.49	0.48
	3	43.21	54.53	0.82	1.45	54.94	41.63	1.36	2.07	45.30	52.01	1.26	1.43	58.93	34.35	1.56	5.15
	4	0.09	1.38	0	98.53	0.52	1.66	0.00	97.82	0.09	1.36	0	98.55	3.79	1.81	0.04	94.36
		Economic															
Rank position	1	0.35	2.05	97.36	0.24	0	9.78	82.31	7.91	0	2.13	94.55	3.31	0.09	38.11	41.89	19.92
	2	8.31	63.81	2.27	25.60	0	39.16	14.59	46.25	0.13	23.97	4.90	70.99	1.78	29.67	35.83	32.73
	3	19.94	19.62	0.30	60.14	0.42	50.71	3.03	45.85	7.25	66.67	0.38	25.70	11.31	30.52	21.43	36.74
	4	71.39	14.52	0.07	14.02	99.58	0.35	0.07	0	92.61	7.22	0.17	0	86.83	1.71	0.85	10.62
		Social															
Rank position	1	7.12	89.52	0	0.00	7.12	89.52	0	0	7.12	89.52	0	0	6.90	88.24	1.72	0.00
	2	92.88	10.48	0	0.00	92.73	10.48	0.15	0	92.88	10.48	0	0	80.70	10.70	11.48	0.04
	3	0	0	99.11	0.65	0.15	0	98.96	0.65	0	0	99.11	0.65	12.14	1.04	85.93	0.89
	4	0	0	0.89	99.35	0	0	0.89	99.35	0	0	0.89	99.35	0.27	0.02	0.88	99.07

S.13 Average SMAA scores per sustainability dimension for different weighting schemes. SC – scenario, ROCW – rank order centroid weights, REW – rank exponent weights, and SRW – stochastic random weights.

		SC1	**SC2**	**SC3**	**SC4**
Environmental	**ROCW**	0.284	0.048	2.334	-2.666
	REW flat	-0.048	0.253	2.292	-2.496
	REW steep	0.219	0.118	2.285	-2.622
	SRW	-0.199	0.331	2.297	-2.428
Economic	**ROCW**	-0.652	-0.157	0.952	-0.143
	REW flat	-0.993	0.150	0.600	0.243
	REW steep	-0.825	-0.140	0.796	0.170
	SRW	-1.080	0.417	0.517	0.146
Social	**ROCW**	1.152	1.899	-0.892	-2.159
	REW flat	0.961	1.871	-0.644	-2.188
	REW steep	1.047	1.887	-0.755	-2.179
	SRW	0.976	1.872	-0.667	-2.181

S.14 Histograms and Kernel density plots of environmental SMAA results for different weighting schemes. SC – scenario, ROCW – rank order centroid weights, REW – rank exponent weights, and SRW – stochastic random weights.



S.15 Average integrated SMAA scores for different weighting schemes and preference structures. SC – scenario, EW – equal weights, and SRW – stochastic random weights.

		SC1	SC2	SC3	SC4
Integrated sustainability	**EW, TYPE 1**	0.627	-1.060	-1.465	1.899
	EW, TYPE 2, p = 1 q = 0	0.650	-1.240	-1.628	2.219
	EW, TYPE 2, p = 2 q = 1	0.469	-0.695	-1.028	1.254
	SRW, TYPE 1	0.628	-1.059	-1.468	1.898
	SRW, TYPE 2, p = 1 q = 0	0.646	-1.241	-1.625	2.220
	SRW, TYPE 2, p = 2 q = 1	0.469	-0.694	-1.029	1.253

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