SUPPLEMENTARY INFORMATION

Renewable carbon opportunities in the production of succinic acid applying attributional and consequential modelling.

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Summary

This document contains the supplementary information and results of the paper entitled "Renewable carbon opportunities in the production of succinic acid applying attributional and consequential modelling". The Life cycle inventory (LCI) tables for the system under study (production of 1 kg of biobased succinic acid from SSL), the results for succinic acid market growth and marginal mix estimations as well as the inventories for Consequential LCA are detailed. Figures presenting further results, complementary to the main manuscript are depicted here as well.

1. System boundary description

The detailed description of each subsystem included within the scope of the analysis is provided below.

SS1. Eucalyptus woodchips. Short rotation *Eucalyptus globulus* wood is the raw material processed in the paper pulping facility. This subsystem includes seedling activities, planting, weed control and fertilizing, felling, forwarding, harvesting and wood chipping. The production yield was considered as 10.1 m^3/ (year ha) in the region of Galicia (Spain) [1,2] and a carbon content of 31.7% [3].

SS2. Pulp and paper industry. In this subsystem, eucalyptus chips were transported over 100 km from the wood production site through road transportation (lorry). Bisulfite pulping was the processing technology considered for pulp production, yielding the SSL stream used as sugar nutrient source in subsequent subsystems. Calcium bisulfite ($Ca (HSO_3)_2$) is the main the cooking chemical utilized for the digestion of wood. It is produced on site, with liquid sulfur, burned to obtain SO_2 and put in contact in an absorption column with an aqueous calcium carbonate solution. The digester, which is operated at 145°C for 4 hours requires 4 metric tons of liquor per ton of wood chips. The contents of the digester are transferred to a blow tank, in which vapors —mainly SO_2— are recovered and recycled. The pulped wood is washed in countercurrent with water. Two main streams are obtained after the washing cycle. First, the pulp which is further processed and bleached to obtain paper (out of the scope of this work). Second, the liquor or SSL, which is a stream containing dissolved sugars and lignosulfonates [4]. Emissions to water and air from the pulping section of the paper producing facility were considered [5].

SS3. Pretreatment. The SSL stream from SS2 —the pulp and paper facility— contains solubilized lignin in the form of lignosulfonates and sugars (mostly xylose, galactose and glucose). Thus, pretreatment is required prior to the fermentation section in order to remove the lignosulfonates (which act inhibitory to microbial growth) and to obtain a lignin-free stream rich in sugars. SSL is diluted with water in a 1:3.5 ratio. Successively, lignosulfonates are separated through nanofiltration (800 Da) with a 97% removal efficiency [6]. Nanofiltration also served as sterilization procedure for the SSL stream prior to fermentation.

SS4. Sterilization. This subsystem includes the mixing of nitrogen sources and minerals (NaH_2PO_4, Na_2HPO_4, NaCl, $MgCl_2$, $CaCl_2$) that are necessary for the fermentation, and inoculum preparation. The nutrients are sterilized via continuous sterilization at 140°C using low pressure stream at 160°C.

SS5. Fermentation. In this study, fermentation was operated in fed-batch and continuous mode, with the bacterial strain *Basfia succiniciproducens* for an annual succinic acid production capacity of 30 kt. The fermentation was conducted at 37°C with agitation and maintaining pH at 6.7 with NaOH. For the fed-batch mode, the final SA concentration was 33.8 g/L with a productivity of 0.56 g/(L·h) and yield 0.58 $g_{SA}/g_{SSL\ Sugar}$ [6]. The respective values for continuous fermentations were 19.6 g/L, 0.79 g/(L·h) and 0.49 $g_{SA}/g_{SSL\ Sugar}$ at a dilution rate of 0.04 h^{-1} [7].

SS6. Downstream. bio-SA was recovered from the fermentation broth in a series of steps in the downstream section. First the bacterial biomass was separated and discarded through a centrifuge. The active carbon columns allow the decolorization and removal of impurities from the solution. Cationic resins were used for the acidification of organic acid salts (e.g. acetate, formate, lactate) into their corresponding acid forms. The rich in organic acids stream was concentrated in an evaporator system where part of the volatile organic acids are removed (formic acid 89% and acetic acid 76%). The concentrated liquid was driven to a crystallizer where the succinic acid was separated in the form of crystals. The SA crystals are removed and dried through rotary filter and spray drier units, respectively.

Business as usual (BAU) scenarios. The fossil production of SA considered for benchmark was the production of SA from maleic anhydrite hydrogenation in liquid phase and metallic catalysts. The process includes SA hydration, crystallization, filtration, and drying steps [8]. The BAU biobased alternative was the production of SA from sorghum saccharification and fermentation by anaerobic bacteria. In this process ammonium sulfate is produced as co-product [9]. ç

2. Details of the methodology

2.1 Attributional LCA

For SS1 and SS2 the impacts were assigned to the two main products exiting SS2, the pulp and the pre-processed SSL. For economic allocation, since we are dealing intermediate products, it was estimated that the economic value of SSL and pulp was that of their further processed end products (i.e., fermentable sugars and dissolving pulp respectively) [10,11].

In SS3 (nanofiltration) the allocation was performed among the two main valuable products obtained, pre-treated SSL —which would be one of the main substrates carried forward into fermentation— and lignosulfonates. The economic value of lignosulfonates is based in their potential application as plasticizing additives in cement mixtures [12].

Especially in the case of CO_2, which experiences a shift from emission to input flow (technical flow), the consideration of allocation rather than considering zero background emissions is pertinent, as to account correctly for emissions in CCU. In this case, as in every input for LCA its background impacts in a cradle-to-gate perspective should be accounted for. Allocation was performed between CO_2 and clinker [13] and CO_2 and bioethanol [14] in the fossil and biogenic CCU scenarios [15]. For economic allocation, the cost of capturing CO_2 from diverse point sources, evidently differs, which was considered [16]. The BAU biobased scenario impacts have been allocated to succinic acid and ammonium sulfate respectively, for comparability reasons [17,18].

2.2 Consequential LCA

The first step in C-LCA is to determine the reference product and co-products of the system. The products of the system under study are SA and lignosulfonates. Lignosulfonates are the dependent co-product, since their revenue does not exceed 80% of the total revenue of the system following the identification of the determining product criterion. Therefore, the system is expanded to include the co-product (lignosulfonates) which is considered as an avoided burden of another market (i.e., plasticizer additive in the cement industry) [19]. The production of SA from sorghum as the first-generation biomass conversion scenario (BAU) produces ammonium sulfate, considered as avoided product in C-LCA [8].

The case of SSL displays a constrained market meaning that it is a dependent by product of the pulp and paper industry. The system boundaries are thus expanded to include its use or treatment. Analyzing its current market, bioethanol is the main product derived from SSL — stream rich in sugars apt for any fermentation. However, the shift of producing SA from SSL rather than the state-of-the-art production of bioethanol results in the need to compensate the bioethanol produced by SSL with the corresponding marginal technology that will be able to absorb the demand. The identification of marginal suppliers was performed on the basis of the 5-step procedure developed by Weidema et al. [20] resulting in the identification of the suppliers that would be able to change their production capacity in response to a change in demand. In a growing market such as that of bioethanol, the marginal technology is that with the greatest historical production growth (i.e., bioethanol produced from maize) [21]. The sugar contents in SSL and sugar consumption patterns for the production of bioethanol were considered for the estimation of the amount of bioethanol per functional unit that should be compensated [6,22].

Obtaining CO_2 from point sources, to produce bio-SA from SSL would lead to an intrinsic change of the clinker and bioethanol industries. These are industries with the feasibility to absorb the increase of demand of CO_2, however they would experience a shift in which the current BAU production with carbon emissions to the environment will be substituted by an identical production with a carbon capture plant and with the consequent elimination of 90% of the carbon emissions to the environment [23]. The result, in our system, is a process substitution in which the reduction or increment of indirect and direct emissions will be accounted as a difference and included in the inventory.

The production of SA with SLL as carbon source will lead to displacing the BAU production methods in the current market. The affected suppliers in this study are part of the selection of a marginal supply mix obtained by extrapolating available market trends. The use of a marginal supply mix makes sense for newer markets with less availability of data or increased uncertainty due to their bio-based nature, which makes difficult to predict their evolution. The SA market is expected growth with an annual rate of anywhere from 7 to 49% in the next years [24–27].

3. Life cycle inventory

Table S1. Inventory for silviculture activities (SS1) per m^3 of eucalyptus wood and their CO_2 uptake estimation [1–3]

SS1. Production of eucalyptus wood chips (1m^3)		
Item	***Amount***	***Units***
Mass inputs from technosphere		
Land use (forest extensive occupation)	0.091	ha·a
E. globulus stems	22	stems
Diesel	0.68	kg
Petrol	7.78	g
Lubricants	30	g
Herbicide (glyphosate)	87	g
Ternary fertilizer (16%N 8%P_2O_5 12%K_2O)	0.14	kg
Diammonium phosphate (18%N 46%P_2O_5)	1.33	kg
Lorry 3.5 t	0.52	tkm
Inputs from nature		
CO_2 uptake from Eucalyptus Woodchips	1.16	kg CO_2/kg wood
Outputs to technosphere		
Wood chips	1	m^3
Emissions to air		
SO_2	7.26	g
NO_x	40	g
CO_2	2.38	kg
CO	9.17	g
VOC	5.4	g
N_2O	24	g
Pentane	0.24	g
NMVOC	24	mg
CH_4	97	mg
Particulates	0.89	g
N_2	70	g
NH_3	59	g
Emissions to water		
NO_3^-	1.51	kg
PO_4^-	12	g

Table S2. Inventory for the pulping (SS2) with calcium bisulfite of wood (in a pulp and paper factory (no bleaching or further pulp processing included) [4,5]

SS2. Pulp and paper factory (per kg SSL)		
Item	***Amount***	***Units***
Mass inputs from technosphere		
Eucalyptus woodchips	$9.99\cdot10^{-4}$	m^3
Sulfur	$1.20\cdot10^{-2}$	kg
Calcium carbonate	$1.18\cdot10^{-2}$	kg
Process water	12.19	kg
NaOH	$3.64\cdot10^{-4}$	kg
Transport (lorry)	105	kgkm
Energy inputs from technosphere		
Electricity	$6.55\cdot10^{-2}$	kWh
Steam	0.26	kg
Outputs to technosphere		
SSL	1.00	kg
Pulp	0.78	kg
Emissions to air		
Water (vent)	$4.73\cdot10^{-3}$	kg
CO_2 (vent)	$2.91\cdot10^{-3}$	kg
SO_2 (vent)	$8.00\cdot10^{-6}$	kg
NaOH (vent)	$4.73\cdot10^{-4}$	kg
Steam out	$7.03\cdot10^{-2}$	kg
Emissions to water		
COD	$4.10\cdot10^{-3}$	kg
BOD	$1.67\cdot10^{-3}$	kg
Total P	$6.39\cdot10^{-4}$	kg
Total N	$3.62\cdot10^{-3}$	kg

Table S3. Inventory for the pretreatment of SSL (SS3), through nanofiltration obtaining lignosulfonates as co-products, continuous operation [6]

SS3. Pretreatment (per kg SA)		
Item	***Amount***	***Units***
Energy inputs from technosphere		
Electricity filtration	0.01	kWh
Outputs		
SSL	4.25	kg
Lignosulfonates	2.15	kg

Table S4. Inventory for the pretreatment of SSL (SS3) through nanofiltration, obtaining lignosulfonates as co-products, fed batch operation [6]

SS3. Pretreatment (per kg SA)		
Item	***Amount***	***Units***
Energy inputs from technosphere		
Electricity filtration	0.06	kWh
Outputs to process and technosphere		
SSL	4.25	kg
Lignosulfonates	2.15	kg

Table S5. Inventory for the sterilization of inputs to the fermentation (SS4), continuous operation [7]

SS4. Sterilization (per kg SA)		
Item	***Amount***	***Units***
Energy inputs from technosphere		
Steam for sterilization	0.27	kg

Table S6. Inventory for the sterilization of inputs to the fermentation (SS4), fed batch operation [7]

SS4. Sterilization (per kg SA)		
Item	***Amount***	***Units***
Energy inputs from technosphere		
Steam for sterilization	0.20	kg

Table S7. Inventory for continuous fermentation for the production SA (SS5)

SS5. Fermentation (per kg SA)		
Item	***Amount***	***Units***
Mass inputs from technosphere		
Water	1.00	kg
Yeast extract	0.25	kg
NaH_2PO_4x H_2O	$5.91 \cdot 10^{-2}$	kg
Na_2HPO_4	$1.58 \cdot 10^{-2}$	kg
NaCl	$5.09 \cdot 10^{-2}$	kg
$MgCl_2$ x 6 H_20	$1.02 \cdot 10^{-2}$	kg
$CaCl_2$ x 2 H_2O	$1.02 \cdot 10^{-2}$	kg
NaOH	1.00	kg
CO_2	0.37	kg
Process water cooling	4.00	kg
Energy inputs from technosphere		
Electricity agitation	1.43	kWh
Electricity cooling	$3.10 \cdot 10^{-2}$	kWh

Table S8. Inventory for fed batch fermentation for the production SA (SS5)

SS5. Fermentation		
Item	***Amount***	***Units***
Mass inputs from technosphere		
Water	0.59	kg
Yeast extract	$1.48 \cdot 10^{-1}$	kg
$MgCO_3$	$1.48 \cdot 10^{-1}$	kg
NaH_2PO_4x H_2O	$3.40 \cdot 10^{-2}$	kg
Na_2HPO_4	$9.20 \cdot 10^{-3}$	kg
NaCl	$2.96 \cdot 10^{-2}$	kg
$MgCl_2$ x 6 H_20	$5.90 \cdot 10^{-3}$	kg
$CaCl_2$ x 2 H2O	$5.90 \cdot 10^{-3}$	kg
NaOH	1.20	kg
CO_2	0.30	kg
Process water cooling	4.00	kg
Energy inputs from technosphere		
Electricity agitation	2.07	kWh
Electricity cooling	$3.10 \cdot 10^{-2}$	kWh

Table S9. Inventory for the separation sequence of SA in continuous operation (SS6)

SS6. Downstream (per kg SA)		
Item	***Amount***	***Units***
Mass inputs from technosphere		
Activated carbon, columns	$1.20 \cdot 10^{-3}$	kg
Resin, ion exchange	$4.00 \cdot 10^{-4}$	kg
HCl	0.90	kg
Energy inputs from technosphere		
Electricity centrifugation	$5.40 \cdot 10^{-2}$	kWh
Electricity evaporation	1.60	kWh
Electricity crystallization	0.19	kWh
Outputs to technosphere		
Wastewater	1.45	kg
Succinic acid	1	kg
Waste to treatment		
Bacterial biomass to incineration	0.12	kg
Spent activated carbon	$1.20 \cdot 10^{-3}$	kg
Spent ion exchange resin	$4.00 \cdot 10^{-4}$	kg

Table S10. Inventory for the separation sequence of SA in fed batch operation (SS6)

SS5. Downstream		
Item	***Amount***	***Units***
Mass inputs from technosphere		
Activated carbon, columns	$1.20\cdot10^{-3}$	kg
Resin, ion exchange	$4.00\cdot10^{-4}$	kg
HCl	1.1	kg
LP steam evaporation	0.29	kg
Energy inputs from technosphere		
Electricity centrifugation	$3.16\cdot10^{-2}$	kWh
Electricity evaporation	0.94	kWh
Electricity crystallization	0.19	kWh
Outputs to technosphere		
Wastewater	1.74	kg
Succinic acid	1	kg
Waste to treatment		
Bacterial biomass to incineration	0.15	kg
Spent activated carbon	$1.20\cdot10^{-3}$	kg
Spent ion exchange resin	$4.00\cdot10^{-4}$	kg

Table S11. Inventory for the capture of CO_2 from the production of clinker assuming 90% capture rate (SS5) [28]

Carbon capture and utilization (fossil alternative)		
CO_2 from fossil point source, long-term supplier, cement industry (per ton clinker)		
Item	***Amount***	***Units***
Mass inputs from technosphere		
Clinker (no CC)	1.00	kg
Ammonia	$2.00\cdot10^{-3}$	kg
MEA	$2.60\cdot10^{-3}$	kg
Limestone	$1.40\cdot10^{-3}$	kg
Energy inputs from technosphere		
Electricity	$7.00\cdot10^{-5}$	MWh
Heat	$2.25\cdot10^{-3}$	GJ
Outputs to technosphere		
Clinker (with CC)	1	kg
CO_2 (90% captured)	0.76	kg
Emissions to air		
CO_2 (10% not captured)	0.084	kg

Table S12. Inventory for the capture of CO_2 from the production of bioethanol assuming 90% capture rate (SS5) [29]

Biobased carbon capture and utilization		
CO_2 from biogenic point source, near-term supplier, bioethanol fermentation		
Item	***Amount***	***Units***
Mass inputs from technosphere		
Bioethanol from wood (no CC)	1.00	kg
Energy inputs from technosphere		
Electricity	0.11	kwh/kg CO_2
Outputs to technosphere		
Bioethanol (with CC)	1	kg
CO_2 (90% captured)	1.16	kg
Emissions to air		
CO_2 (10% not captured)	0.13	kg

Table S13. Inventory for the petrochemical production of SA used as business as usual (fossil BAU) [8]

Petrochemical SA (1kg)		
Item	***Amount***	***Units***
Mass inputs from technosphere		
Maleic anhydride	0.89	kg
Hydrogen	0.25	kg
Water	0.30	kg
Nitrogen	$7.29 \cdot 10^{-2}$	kg
Palladium catalyst	$1.0 \cdot 10^{-5}$	kg
Natural gas	0.10	kg
Energy inputs from technosphere		
Electricity	0.36	kWh
Outputs to technosphere		
Succinic acid	1	kg
Waste to treatment		
Waste (generic)	0.32	kg

Table S14. Inventory for the biobased production of SA used as business as usual (biobased BAU) [9]

First generation SA (1kg)		
Item	***Amount***	***Units***
Mass inputs from nature		
CO_2	2.01	kg
Cooling water	1.23	m^3
Mass inputs from technosphere		
Sorghum grain	1.66	kg
Sulfuric acid	1.11	kg
Ammonia	0.41	kg
Tap Water	1.67	kg
Ultrapure water	25.3	kg
Glucose	$1.30{\cdot}10^{-2}$	kg
Energy inputs from technosphere		
Electricity	2.67	kWh
Heat	14.77	MJ
Outputs to technosphere		
Succinic acid	1	kg
Ammonium sulfate	1.49	kg
Waste to treatment		
Wastewater	$1.1{\cdot}10^{-2}$	m^3
Biowaste (incineration)	$8.2{\cdot}10^{-1}$	kg
Sorghum bagasse	$3.95{\cdot}10^{-1}$	kg
Emissions to air		
Water	2.72	kg
Volatile organic compounds	$2.00{\cdot}10^{-3}$	kg
Carbon monoxide	$1.50{\cdot}10^{-2}$	kg
Nitrogen oxides	$5.00{\cdot}10^{-3}$	kg
Particulates μm<10	$1.00{\cdot}10^{-3}$	kg
Ammonia	$1.72{\cdot}10^{-4}$	kg
Lead	$5.20{\cdot}10^{-6}$	kg
Sulfuric acid	$8.06{\cdot}10^{-5}$	kg

Table S15. Prices for outputs in the life cycle for the production of SA (Considered in economic allocation calculations)

Product	**Price**	**Unit**	**Average €/kg**	**Reference**
Bioethanol	0.47	$/l	0.524	[14]
Clinker	37	€/t	0.0370	[13]
CO_2 from clinker	26-42	$/ton	0.0299	[16]
CO_2 from ethanol	14	$/ton	0.0123	[16]
Lignosulfonates	300	$/ton	0.240	[12]
SSL (assuming price of fermentable sugars- xylose)	0.4	$/kg	0.320	[10]

Pulp (assuming price of dissolving pulp)	1350	€/t	1.35	[11]
Ammonium sulfate	0.137	\$/kg	0.121	[17]
Succinic acid			2.8	[18]

Table S16. Economic and mass allocation factors in A-LCA

Subsystem	Outputs	Mass allocation (%)	Economic allocation (%)
SS2	Pulp	43.90	84.35
	SSL	56.10	15.65
SS3	SSL rich in sugars	66.41	72.49
	Lignosulfonates	33.59	27.51
SS5 (CO_2 from biogenic point emission source)	Bioethanol	46.20	97.30
	CO_2	53.80	2.66
SS5 (CO_2 from fossil point emission source)	Clinker	57.00	62.10
	CO_2	43.00	37.90
BAU biobased SA	SA	40.20	93.96
	Ammonium sulfate	59.80	6.04

4. Market trends and marginal mixes for SA

Table S17. Historic market data for SA production volume

Year		1990[a]	2010[b,c]	2011[d]	2015[d]
Fossil	(ton/year)	17,000	25,000	25,000	25,000
Biobased 1st generation	(ton/year)	1	1,250	10,000	180,000
Total	(ton/year)	17,001	26,250	35,000	205,000

a [26]
b [30]
c [9]
d [8]

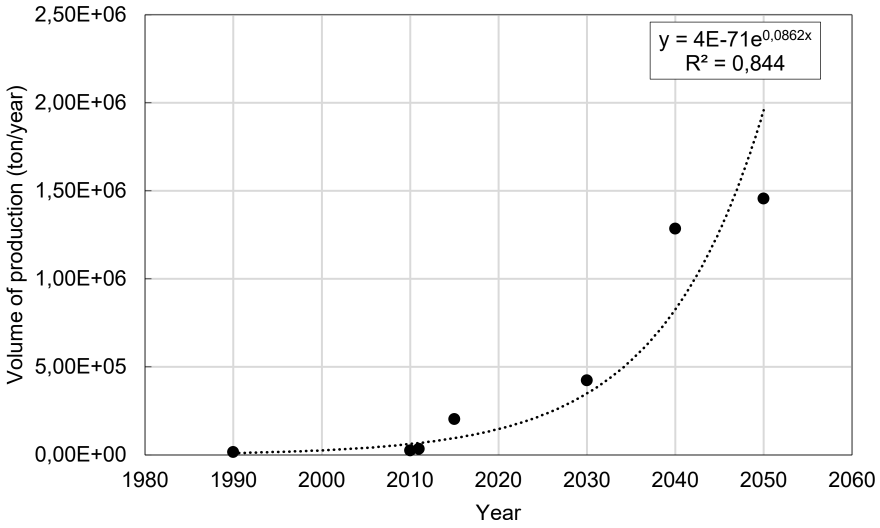

Figure S1. Estimated projection of growth for succinic acid production from data in table S17

Table S18. Current mix of production of SA, year 2015

	Current mix
Fossil	12%
Biobased 1st generation	88%

Table S19. Marginal mix estimation for short-term scenarios in timeline 1 (LT1 scenarios)

	Fossil	**Biobased 1st generation**
Annual trend	1.88	719,996
Technology lifetime	40	40
Capital replacement rate (%)	-2.5	-2.5
Net annual trend (%)	4.38	719,999
Net annual change	7,450	7,200
Marginal mix (%)	50.85	49.15

Table S20. Marginal mix estimation for short-term in timeline 2 (LT2 scenarios)

	Fossil	**Biobased 1st generation**
Annual trend	1.88	2,860
Technology lifetime	40	40
Capital replacement rate (%)	-2.50	-2.50
Net annual trend (%)	4.38	2,863
Net annual change	7,450	35,781
Marginal mix (%)	17.23	82.77

Table S21. Marginal mix estimation long-term scenarios (LT)

	Fossil	**Biobased 1st generation**
Annual trend	0	2,860
Technology lifetime	N/A	40
Capital replacement rate (%)	N/A	-2.5
Net annual trend (%)	N/A	28,623
Net annual change	N/A	35,781
Marginal mix (%)	0	100

5. Life cycle inventory Consequential LCA

Table S22. Current scenario (no change in current mix of SA)

Current scenario	Value	Units
SA fossil (12%) + SA biogenic (88%)	1	kg
Avoided ammonium sulfate	1.31	kg

Table S23. Consequential LCA inventory for short term scenarios (TL1)

Short term scenario, B-ST-TL1	Value	Units
SA (present study, no allocations, biobased CO_2)	1	kg
Displaced ethanol (from corn)	0.322	kg/kg SA
Substituted bioethanol industry (now with CC)	0.296	kg/kg SA
SA avoided (50.9% fossil, 49.1% biobased)	1	kg
Lignosulfonates (avoided additives-plasticizer for cement)	2.15	kg/kg SA
Short term scenario, F-ST-TL1		
SA (present study, no allocations, fossil CO_2)	1	kg
Displaced ethanol (from corn)	0.322	kg/kg SA
Substituted clinker industry (now with CC)	0.494	kg/kg SA
SA avoided (50.9% fossil, 49.1% biobased)	1	kg
Lignosulfonates (avoided additives-plasticizer for cement)	2.15	kg/kg SA

Table S24. Consequential LCA inventory for short term scenarios (TL2)

Short term scenario, B-ST-TL2	Value	Units
SA (present study, no allocations, biobased CO_2)	1	kg
Displaced ethanol (from corn)	0.322	kg/kg SA
Substituted bioethanol industry (now with CC)	0.296	kg/kg SA
SA avoided (17.2% fossil, 82.8% biobased)	1	kg
Lignosulfonates (avoided additives-plasticizer for cement)	2.15	kg/kg SA
Short term scenario, F-ST-TL2		
SA (present study, no allocations, fossil CO_2)	1	kg
Displaced ethanol (from corn)	0.3216	kg/kg SA
Substituted clinker industry (now with CC)	0.4940	kg/kg SA
SA avoided (17.2% fossil, 82.8% bio)	1	kg
Lignosulfonates (avoided additives-plasticizer for cement)	2.15	kg/kg SA

Table S25. Consequential LCA inventory for long term scenarios (LT)

Long term scenario, B-LT	Value	Units
SA (present study, no allocations, biobased CO_2)	1	kg
Displaced ethanol (from corn)	0.322	kg /kg SA
Displaced bioethanol industry (now with carbon capture)	0.296	kg /kg SA
SA avoided (0% fossil, 100% bio)	1	kg
Lignosulfonates (avoided additives-plasticizer for cement)	2.15	kg
Long term scenario, F-LT		
SA (present study, no allocations, biobased CO_2)	1	kg
Displaced ethanol (from corn)	0.322	kg /kg SA
Displaced clinker industry (now with CC)	0.494	kg /kg SA
SA avoided (0% fossil, 100% bio)	1	kg
Lignosulfonates (avoided additives-plasticizer for cement)	2.15	kg

6. Results

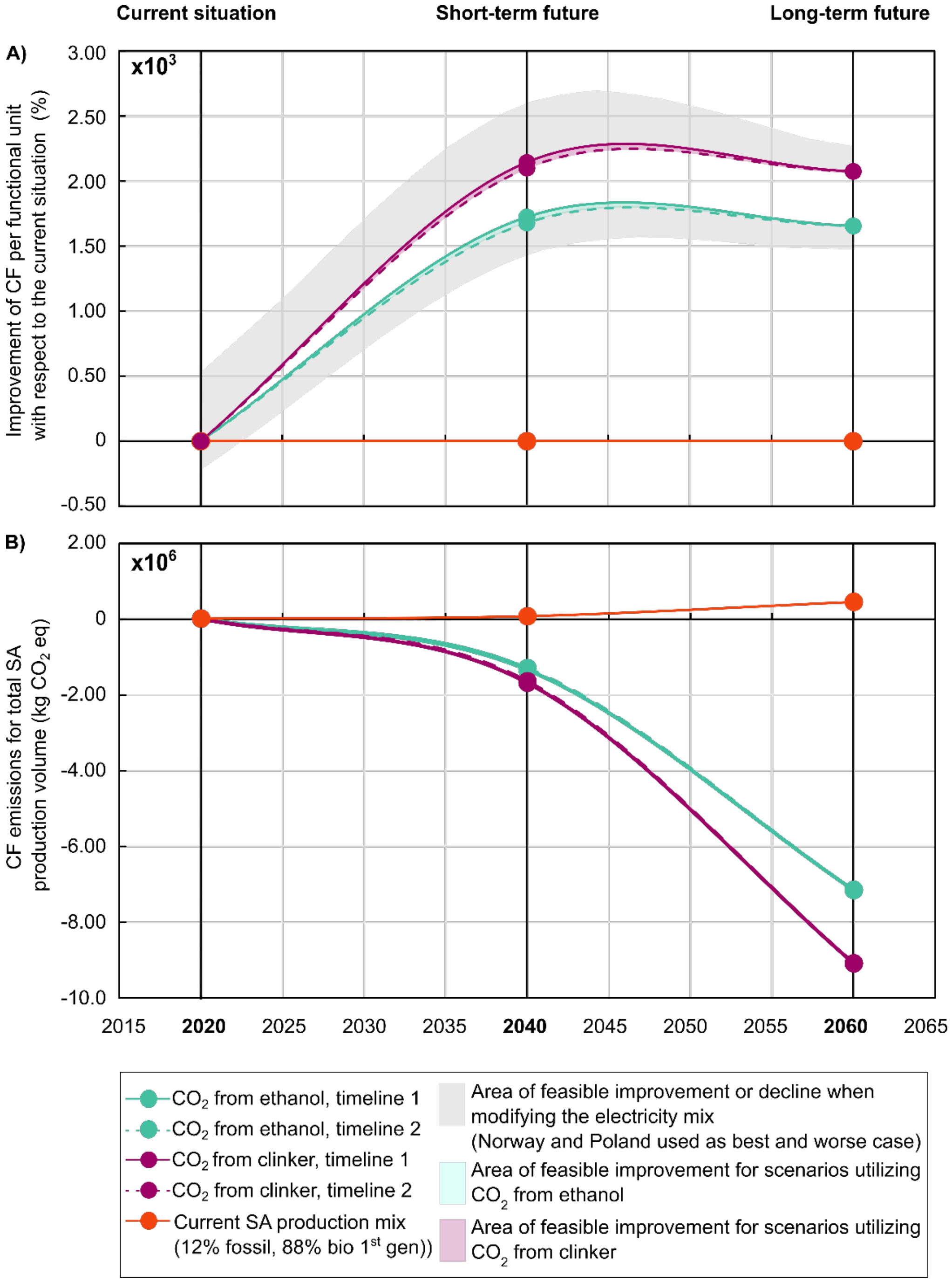

Figure S2. Projection of C-LCA impacts in Carbon Footprint (CF) to 20 and 40 years from the current situation. SA is produced in fed-batch operation. A) Displays the percent improvement of the CF with respect to the current SA scenario per functional unit B) Displays the total CF of SA market considering a growth in the SA production volume

Percent-improvement calculations for consequential values

The maximum value for the percent-improvement in each CCU scenario corresponds to that of TL1 (short-term, timeline 1), which are, for fossil and biogenic CO_2 the best scenarios with respect to the BAU. The percent-improvement was obtained as follows:

$$\text{Improvement}\ (\%) = \frac{\left(\frac{\text{CF}}{\text{FU}}\right)_{\text{BAU}} - \left(\frac{\text{CF}}{\text{FU}}\right)_{\text{SCEN}}}{\left(\frac{\text{CF}}{\text{FU}}\right)_{\text{BAU}}} \times 100\% \qquad \text{Eq. 1}$$

Where $\frac{\text{CF}}{\text{FU}}$ is the carbon footprint per functional unit for each scenario, BAU is the business-as-usual case (current scenario), and SCEN represents any of the scenarios in the current study. Regarding the results from Eq. 1 presented in the main manuscript:

For 1465%, SCEN= F-ST-TL1

For 1023%, SCEN= B-ST-TL1

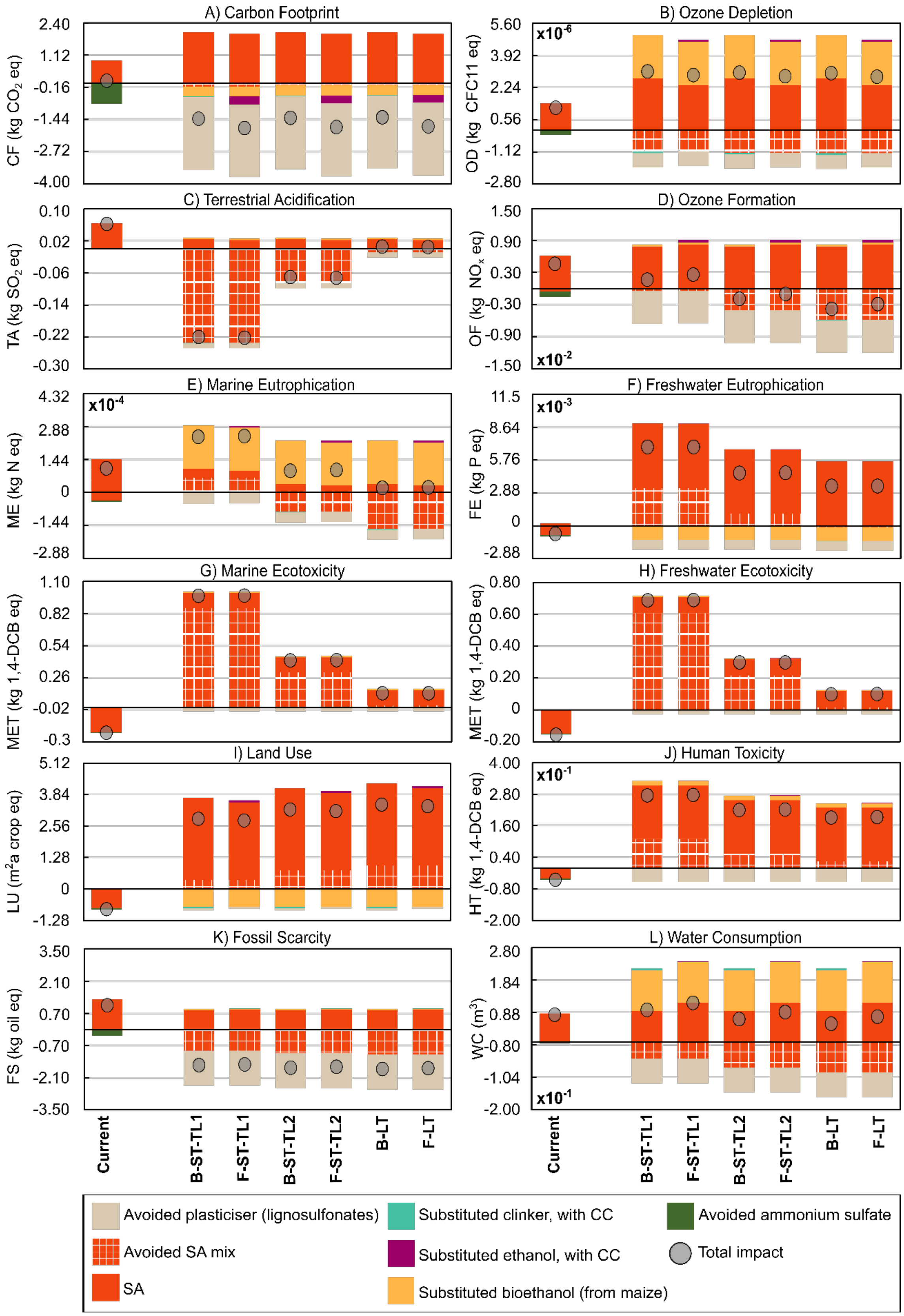

Figure S3. Comparative evaluation and breakdown of environmental profiles through C-LCA for SA produced in fed-batch operation. A) Carbon footprint B) Ozone depletion C) Terrestrial acidification D) Ozone formation E) Marine eutrophication F) Freshwater eutrophication G) Marine ecotoxicity H) Freshwater ecotoxicity I) Land use J) Human toxicity K) Fossil scarcity L) Water consumption.

References

[1] M. Morales, G. Aroca, R. Rubilar, E. Acuña, B. Mola-Yudego, S. González-García, Cradle-to-gate life cycle assessment of Eucalyptus globulus short rotation plantations in Chile, J. Clean. Prod. 99 (2015) 239–249. doi:10.1016/j.jclepro.2015.02.085.

[2] S. González-García, M.T. Moreira, G. Feijoo, R.J. Murphy, Comparative life cycle assessment of ethanol production from fast-growing wood crops (black locust, eucalyptus and poplar), Biomass and Bioenergy. 39 (2012) 378–388. doi:10.1016/j.biombioe.2012.01.028.

[3] Phyllis2 ECN, ECN Phyllis classification, wood, eucalyptus, (1998). https://phyllis.nl (accessed July 22, 2020).

[4] S. Chen, T. Spink, A. Gao, Aspen Modeling of the NARA Conversion Processes, 2016. https://nararenewables.org/documents/2016/10/aspen-modeling-of-the-nara-conversion-processes.pdf/.

[5] I.S. Modahl, A. Brekke, C. Valente, Environmental assessment of chemical products from a Norwegian biorefinery, J. Clean. Prod. 94 (2015) 247–259. doi:10.1016/j.jclepro.2015.01.054.

[6] C. Pateraki, D. Ladakis, L. Stragier, W. Verstraete, I. Kookos, S. Papanikolaou, A. Koutinas, Pretreatment of spent sulphite liquor via ultrafiltration and nanofiltration for bio-based succinic acid production, J. Biotechnol. 233 (2016) 95–105. doi:10.1016/j.jbiotec.2016.06.027.

[7] D. Ladakis, K. Michailidi, A. Vlysidis, A. Koutinas, I.K. Kookos, Valorization of spent sulphite liquor for succinic acid production via continuous fermentation system, Biochem. Eng. J. 137 (2018) 262–272. doi:10.1016/j.bej.2018.05.015.

[8] J.M. Pinazo, M.E. Domine, V. Parvulescu, F. Petru, Sustainability metrics for succinic acid production: A comparison between biomass-based and petrochemical routes, Catal. Today. 239 (2015) 17–24. doi:10.1016/j.cattod.2014.05.035.

[9] H.I. Moussa, A. Elkamel, S.B. Young, Assessing energy performance of bio-based succinic acid production using LCA, J. Clean. Prod. 139 (2016) 761–769. doi:10.1016/j.jclepro.2016.08.104.

[10] D. Parra-Ramírez, A. Martinez, C. Ariel Cardona, Technical and economic potential evaluation of the strain Escherichia coli MS04 in the ethanol production from glucose and xylose, Biochem. Eng. J. 140 (2018) 123–129. doi:10.1016/j.bej.2018.09.015.

[11] R. Nitzsche, A. Gröngröft, J. Köchermann, K. Meisel, H. Etzold, M. Verges, M. Leschinsky, J. Bachmann, B. Saake, S. Torkler, K. Patzsch, B. Rößiger, D. Pufky-Heinrich, G. Unkelbach, Platform and fine chemicals from woody biomass: demonstration and assessment of a novel biorefinery, Biomass Convers. Biorefinery. (2020). doi:10.1007/s13399-020-00769-z.

[12] J. Holladay, J. White, J. Bozell, D. Johnson, Top Value-Added Chemicals from Biomass, 2007. http://www.ntis.gov/ordering.htm.

[13] McKinsey Climate Change Initiative, Carbon Capture & Storage: Assessing the Economics, 2008.

[14] E. Gnansounou, Production and use of lignocellulosic bioethanol in Europe: Current situation and perspectives, Bioresour. Technol. 101 (2010) 4842–4850.

doi:10.1016/j.biortech.2010.02.002.

[15] A. Zimmermann, J. Wunderlich, G. Buchner, L. Müller, K. Armstrong, S. Michailos, A. Marxen, H. Naims, F. Mason, G. Stokes, E. Williams, Techno-Economic Assessment & Life Cycle Assessment Guidelines for CO_2 Utilization, CO2Chem Media and Publishing LTD, 2018.

[16] P. Bains, P. Psarras, J. Wilcox, CO_2 capture from the industry sector, Prog. Energy Combust. Sci. 63 (2017) 146–172. doi:10.1016/j.pecs.2017.07.001.

[17] Independent Commodity Intelligence Services (ICIS), Ammonium Sulfate Market Relatively Stable, (2003). https://www.icis.com/explore/resources/news/2003/07/18/504609/ammonium-sulfate-market-relatively-stable/#:~:text=Mid-June ammonium sulfate pricing,ton in the Pacific Northwest. (accessed March 11, 2021).

[18] M.J. Biddy, C. Scarlata, C. Kinchin, Chemicals from Biomass: A Market Assessment of Bioproducts with Near-Term Potential, NREL Tech. Rep. (2016) 131. doi:10.2172/1244312.

[19] J. Schmidt, Example –soybean and oil co-product system, Consequential LCA. (2014). https://consequential-lca.org/clca/determining-or-dependent-co-products/when-all-co-products-have-alternatives/example-soybean-and-oil-co-product-system/ (accessed March 4, 2021).

[20] B.P. Weidema, N. Frees, A.-M. Nielsen, Marginal Production Technologies for Life Cycle Inventories, Int. J. Life Cycle Assess. 4 (1999) 48–56.

[21] E. Bittencourt Sydney, L.A.J. Letti, S.G. Karp, A.C. Novak Sydney, L. Porto de Souza Vandenberghe, J.C. de Carvalho, A. Lorenci Woiciechowski, A. Bianchi Pedroni Medeiros, V. Thomaz Soccol, C. Ricardo Soccol, Current analysis and future perspective of reduction in worldwide greenhouse gases emissions by using first and second generation bioethanol in the transportation sector, Bioresour. Technol. Reports. 7 (2019) 100234. doi:10.1016/j.biteb.2019.100234.

[22] A.M.R.B. Xavier, M.F. Correia, S.R. Pereira, D. V Evtuguin, Second-generation bioethanol from eucalypt sulphite spent liquor, Bioresour. Technol. 101 (2010) 2755–2761. doi:10.1016/j.biortech.2009.11.092.

[23] N. Thonemann, M. Pizzol, Consequential life cycle assessment of carbon capture and utilization technologies within the chemical industry, Energy Environ. Sci. 12 (2019) 2253. doi:10.1039/c9ee00914k.

[24] J.P. Tan, J. Jahim, S. Harun, T.Y. Wu, Overview of the Potential of Bio-Succinic Acid Production from Oil Palm Fronds, J. Phys. Sci. 28 (2017) 53–72.

[25] R.K. Saxena, S. Saran, J. Isar, R. Kaushik, Production and Applications of Succinic Acid, in: A. Pandey, S. Negi, C.R. Soccol (Eds.), Curr. Dev. Biotechnol. Bioeng. Prod. Isol. Purif. Ind. Prod., Elsevier, Amsterdam, Netherlands, 2017: pp. 601–630. doi:10.1016/B978-0-444-63662-1.00027-0.

[26] N.P. Nghiem, S. Kleff, S. Schwegmann, Succinic Acid : Technology Development and Commercialization, Fermentation. 3 (2017) 1–14. doi:10.3390/fermentation3020026.

[27] J. Garcia-Aguirre, M. Alvarado-morales, I.A. Fotidis, I. Angelidaki, Up-concentration of succinic acid , lactic acid , and ethanol fermentations broths by forward osmosis, Biochem. Eng. J. 155 (2020) 107482. doi:10.1016/j.bej.2019.107482.

[28] D. García-Gusano, D. Garraín, I. Herrera, H. Cabal, Y. Lechón, Life Cycle Assessment of applying CO_2 post-combustion capture to the Spanish cement production, J. Clean. Prod. 104 (2015) 328–338. doi:10.1016/j.jclepro.2013.11.056.

[29] H.B. Carminati, R.D.F.D. Milão, J.L. De Medeiros, O.D.Q.F. Araújo, Bioenergy and full carbon dioxide sinking in sugarcane-biorefinery with post-combustion capture and storage : Techno-economic feasibility, Appl. Energy. 254 (2019) 113633. doi:10.1016/j.apenergy.2019.113633.

[30] P. Gallezot, Conversion of biomass to selected chemical products, Chem. Soc. Rev. 41 (2012) 1538–1558. doi:10.1039/c1cs15147a.