Supporting Information (SI) for:

Target cultivation and financing parameters for sustainable production of fuel and feed from microalgae

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1 Description of models

1.1 Physical models

1.1.1 Cultivation

The cultivation system, for the marine chlorophyte *Desmodesmus* sp. grown under high-nitrogen conditions, was modeled based on the 100ha facility presented in Huntley et al [1] and Beal et al [2], with an average productivity of 23 $g/m^2/day$ in terms of dry weight. The hybrid system consists of a small number of photo-bioreactors (PBR) used to provide inoculum for a series of open ponds. A 30-year facility lifetime and a 90% capacity factor are assumed for the facility.

The water supply with pumping from the ocean is modeled based on the Texas case study of Beal et al [2]. Table S1 summarizes the major daily consumptions of energy and nutrients for the baseline cultivation case, which is the same for the fuel only (hydrothermal liquefaction (HTL)) and for the fuel and feed pathways, without uncertainties. Energy inputs for the dewatering process with a belt filter press, also the same for the two pathways, are also included in this table.

Table S1: daily requirements of energy and materials for the cultivation and dewatering of algae.

Cultivation model component with unit	Baseline value	Daily requirements/production
Electricity for saltwater supply [kWh]	mathematical model detailed in Beal et al [2]	14 724
Electricity to mix PBRs [kWh]	mathematical model detailed in Beal et al [2]	3 493
Electricity to mix open ponds [kWh]	mathematical model detailed in Beal et al [2]	9 388

Electricity for CO_2 compression and transport [kWh]	mathematical model detailed in Beal et al [2]	3 620
Electricity for nutrient mixing [kWh]	mathematical model detailed in Beal et al [2]	157
CO_2 requirement [kg]	1.776 g CO_2/g algae [2]	49 369
Nitrogen requirement [kg]	0.063 g N/g algae [2]	1 380
Phosphorus requirement [kg]	0.0057 g P/g algae [2]	125
Electricity for dewatering (belt filter press) [kWh]	mathematical model detailed in Beal et al [2]	300
Daily algae production after dewatering [kg]	mathematical model detailed in Beal et al [2]	20 200

The model assumes that 94% of the biomass is recovered during harvesting of algae in open ponds. Dewatering increases solids concentration in slurry from 2% to 20%, with a 2% fraction of algae lost during this stage[2]. In the case of the fuel only (HTL) route, the catalytic hydrothermal gasification (CHG) stage allows for recycling part of the nutrients. Information on nutrient recycle, not included in Table S1, is detailed in Section 1.1.2 below.

1.1.2 Processing – fuel only (HTL)

For the fuel only pathway, the dewatered algal slurry is sent to HTL for production of biocrude under high pressure and high temperature (300°C) reaction conditions. The process also produces an aqueous phase containing the remaining organic matter, which undergoes further treatment. Table S2 summarizes the major daily energy and material requirements for the HTL reactor.

Table S2: daily requirements of energy and materials for HTL in the fuel only pathway.

HTL model component with unit	Baseline value	Daily requirements/production
Electricity for HTL [kWh]	0.0835 MJ/kg algae [2]	469
Heat for HTL [MJ]	0.411 MJ/kg algae [2]	8 302
Produced biocrude [kg]	calculated after efficiency detailed below	10 100

The baseline biocrude yield is assumed to be 50% [2], with an oil density of 0.93 kg/L [3]. Regarding nutrient balance, it is assumed that 52% of nitrogen is released into the aqueous phase, and therefore available for further recycling [2], the remaining nitrogen is lost by contaminating the oil phase or it is converted to ammonia during the process. For phosphorus, the amount going to the aqueous phase is assumed to be 75% [4].

After HTL, the aqueous phase undergoes catalytic hydrothermal gasification (CHG) at 350°C and 206 bars, which converts organic matter into a gaseous mixture of CO_2 and CH_4, nutrients and clean water. Water and nutrients can be recycled and therefore sent back to the cultivation system. Table S3 below summarizes the major daily energy and material flows for the CHG reactor.

Table S3: daily requirements and productions of energy and materials for CHG in the fuel only pathway.

CHG model component with unit	Baseline value	Daily requirements/production
Electricity for CHG [kWh]	mathematical model detailed in Beal et al [2]	25

Heat for CHG [MJ]	mathematical model detailed in Beal et al [2]	5 738
Produced syngas by CHG [MJ]	calculated after gas fraction detailed below	111 370
Recovered nitrogen by CHG [kg]	calculated after recovered fraction detailed below	795
Recovered phosphorus by CHG [kg]	calculated after recovered fraction detailed below	86

A baseline syngas yield of 0.5 L/g VS (volatile solids) is assumed for CHG, with average volume fractions of 0.615 for CH_4, 0.016 for H_2, 0.016 for ethane, 0.353 for CO_2 [3,5]. Regarding nutrient recycling, it is assumed that 0.8% of incoming nitrogen is lost as NH_3 during CHG [3], and that all of the incoming phosphorus can be recovered, since no information was available with respect to this particular nutrient.

The syngas is then sent to a combined heat and power (CHP) unit for on-site heat and power production. Heat and power integration is then performed to minimize external heat and electricity inputs using the required power and thermal loads for other process stages, as well as their temperature levels [6]. Table S4 below summarizes the major daily energy productions for CHP.

Table S4: daily productions of energy and materials for CHP for the fuel only pathway.

CHP model component with unit	Baseline value	Daily production
Electricity from CHP [kWh]	calculated after efficiency detailed below	10 608
Heat from CHP [MJ]	calculated after efficiency	48 989

	detailed below	

The electrical and thermal efficiencies of the CHP unit are assumed to be 34% and 44%, respectively, according to the data available in the US-Environmental Protection Agency catalog on CHP engines [7].

1.1.3 Processing – fuel and feed

For the extraction of algal oil from the algal biomass, we modeled the Open Algae wet extraction processes presented Beal et al [2]. It consists in an electro-magnetic lysis of cells, using a lower amount of solvent compared to other oil-extraction processes, heptane in this case. Table S5 below summarizes the major daily energy and material flows for oil extraction and animal feed ingredients production.

Table S5: daily requirements of energy and materials for oil extraction for the fuel and feed pathway.

oil extraction model component with unit	Baseline value	Daily requirements
Electricity for oil extraction [kWh]	0.311 MJ/kg algae [2]	1 745
Heat for oil extraction [MJ]	0.334 MJ/kg algae [2]	6 745
Solvent for oil extraction, including losses [kg]	0.003% loss/g algae [2]	0.505
Produced biocrude [kg]	calculated after efficiency detailed below	5 606
Produced lipid-extracted algae [kg]	calculated after efficiency detailed below	14 595

The required process heat used for extraction is assumed to be supplied by a natural gas boiler. The baseline value for oil extraction efficiency is assumed to be 75% [2]. In addition, no nutrients are recycled, since they are components of the lipid-extracted algae, further used as animal feed ingredients. Although the drying of lipid-extracted algae is accounted for in the heat requirements, further post-processing of the biomass such as pelletizing is not accounted for. The specifications of the final lipid-extracted algal product are currently not defined and remain highly uncertain. For example, if the algal biomass is used in a co-located animal facility, it can retain some of the moisture and require little additional processing. If it has to be shipped and stored, further post-processing such as pelletizing will be required.

1.2 Economic model

The techno-economic model is used to calculate the biocrude minimum selling price, in $/gal. This indicator is calculated using the discounted cash-flow methodology of the National Renewable Energy Laboratory [8, 9]. The major assumptions of the techno-economic model are a discount rate of 10%, a tax rate of 20%, and equity of 40% with a loan term of 10 years at an interest rate of 8%. The maintenance factor, which is the annual percentage of initial capital costs to be attributed every year for equipment maintenance, is assumed to be 3.5%. Equipment is depreciated using a MACRS-7.5 year method. Capital and operating costs have been modeled after the data presented in Beal et al [2]. The baseline values for the two pathways are detailed in Table S6 below, as initial values for capital costs, and per year of operation for operating costs.

Table S6: Capital and operating baseline data without uncertainties for the two pathways: fuel only and fuel and feed pathways. The data are displayed in an aggregated way for the capital costs, per unit, and in an aggregated way for operating costs per type of material or energy flow. The animal feed ingredient sales are displayed as a negative accounting value, since they decrease annual operating costs.

Economic model	Specific cost for	Total cost for fuel	Total cost for fuel

element	base case	only pathway	and feed pathway
Total capital costs, in $			
Land costs	-	242 140	242 140
Cultivation and harvesting system	-	48 784 000	48 784 000
Belt filter press for dewatering	-	1 378 800	1 378 800
HTL reactor	-	4 752 700	0
CHG reactor	-	5 110 400	0
CHP system	-	720 990	0
Oil extraction system	-	0	1 197 636
Utility system (boiler and heat exchangers)	-	135 490	107 580
Operating costs, in $/yr			
Ammonia as N-fertilizer	802 $/MT	187 040	441 480
DAP as P-fertilizer	623 $/MT	33 552	108 800
Carbon dioxide for algal growth	0 $/MT (but the electricity required for compression and transport is accounted for)	0	0
Electricity	0.08 $/kWh	577 500	878 470
Natural gas as heat	0.0225 $/kWh	0	13 852

Solvent	462 $/MT	0	76
Animal feed ingredient sales	587 $/MT	0	(2 814 300)

1.3 Life Cycle Assessment model

The functional unit (FU) of the life cycle assessment (LCA) model, 1 ha of cultivation and processing for facility lifetime – i.e. 30 years, was chosen to avoid co-product allocation in the case of the fuel and feed pathway.

1.3.1 Life Cycle Inventory

The life cycle inventory for the two pathways is based on the data presented in Beal et al [2]. The baseline values for the two pathways are detailed in Table S7 below per functional unit.

Table S7: Life cycle inventories per functional unit (FU) for the base cases without uncertainties for the two pathways: "fuel only" and "fuel and feed". 'EF' stands for elementary flow. The unit of the ecoinvent equivalence is given, as well as the location for which the equivalence is valid (GLO – Global; RoW – Rest of the World without Europe; US – USA; TRE – Texas).

LCI element and unit	ecoinvent equivalence [10]	quantity for fuel only route/FU	quantity for fuel and feed route/FU
N-fertilizer [kg]	ammonia, liquid {RoW} - ammonia production, steam reforming, liquid	54 875	144 420
P-fertilizer [kg]	phosphate fertilizer, as P2O5 {RoW} – diammonium phosphate production	8 276	10 893
electricity [MJ]	electricity, medium voltage {TRE} – electricity voltage transformation from high to medium voltage	7 425 000	11 294 640
heat [MJ]	heat production, natural gas, at boiler modulating >100kW	0	633 240
solvent [kg]	heptane {RoW} – molecular sieve separation of naphtha	0	47
low-density polyethylene [kg]	low density polyethylene {RoW}	61 555	61 555
polyvinyl-chloride [kg]	polyvinylchloride, bulk polymerized {RoW}	220	220
process equipment [unit]	methanol factory {GLO}	0.0017	0.0012

LDPE disposal [kg]	waste polyethylene/polypropylene product {RoW} – treatment of, collection for final disposal	61 5552	61 555
PVC disposal [kg]	waste polyvinylchloride product {RoW}, treatment of, collection for final disposal	220	220
transports [tkm]	transport, freight, lorry 16-32 metric ton, EURO3 {RoW}	12 355	12 355
replaced gasoline [kg]	petrol, low-sulfur {RoW}	-951 970	-528 350
replaced soy in animal feed [kg]	soybean meal {US}	0	-1 027 400
replaced corn in animal feed [kg]	maize grain {US}	0	-342 450
solvent loss [kg]	EF for heptane, air	0	47
land occupation [m2a]	EF for land occupation	22 857	22 857
NO_x in air by CHP [kg]	EF for nitrogen oxides, air	157	0
CO in air by CHP [kg]	EF for carbon monoxide, air	502	0
CH_4 biogenic in air	EF for biogenic methane, air	240	0

by CHP [kg]			
NMVOC in air by CHP [kg]	EF for NMVOC, air	21	0
N_2O in air by CHP [kg]	EF for dinitrogen monoxide, air	26	0
SO_2 in air by CHP [kg]	EF for sulfur dioxide, air	220	0
Avoided fossil CO_2 in air by replaced gasoline[kg]	EF for fossil carbon dioxide, air	-3 019 700	-1 675 900

For the LCA model, to calculate the avoided CO_2 emissions and substituted fossil crude only, we compare the produced biofuel with a gasoline equivalent in terms of energy requirements and emissions. Therefore, for this purpose only we assume a post-processing step after biocrude production, although this stage is not part of our system limits. It is assumed in both pathways that the biocrude is sent to a hydrotreatment unit for green diesel production, with a quality equivalent to fossil diesel. The hydrotreatment efficiency for this conversion stage is assumed to be 0.97 kg diesel/kg oil [11]. The LHV of the produced diesel is then assumed to be 44 MJ/kg and the specific diesel CO_2 emissions that are avoided with the biofuel are assumed to be 3.172 kgCO_2/kg fuel [12]. The hydrotreatment step is included only to calculate the amount of substituted fossil fuel by algal biofuels and its associated avoided CO_2 emissions from combustion. Indeed, accounting for the economics of hydrotreatment would require more information on the quality of produced algal oil by HTL or wet extraction, which is not available.

1.3.2 Life Cycle Impact Assessment

The life cycle impact assessment data for the IMPACT 2002+ method were taken from the ecoinvent database for the four endpoint categories of human health, ecosystem quality, climate change and resources. This method has been chosen since it provides synthetic indicators to ease decision-making while at the same time provides a way of comparing the different impact categories among themselves. The original method uses normalization factors for the European continent, but we used normalization factors for the US context developed by Lautier et al [13]. Table S8 below details the units of each endpoint category and the normalization factors used to convert the data from Europe to the USA. Each normalization factor is worth one point of environmental impact, which corresponds to the yearly impacts generated by an average European or American in the corresponding impact category. This provides a way of comparing the different impact categories among themselves. More details about the conversion from substances of the inventory to midpoint impact categories and from midpoint categories to endpoint categories can be found in the documentation of the impact assessment method [14, 13].

Table S8: Factors for normalizing endpoint impact categories to points of environmental impacts for Impact2002+ method. Values taken from Lautier et al [13]. The abbreviations refer to the the following units: DALY: disability adjusted life years, PDF*m2: potentially depleted fraction of species per meter-square, kgCO_2-eq: kg of CO_2 equivalent for greenhouse gases, MJ primary: MJ of primary energy embedded or required for extraction of minerals

Impact category	Europe norm. factor	USA normalization factor
Human Health [DALY/person/year]	7.88E-03	3.88E-02
Ecosystem Quality [PDF*m^2/person/year]	8.26E+03	4.38E+03
Climate Change [kgCO_2-eq/person/year]	1.05E+04	2.20E+4

Resources [MJ primary/person/year]	7.72E+04	2.03E+05

2 Uncertain parameters

2.1 Foreground uncertainty

The probability distribution functions used to describe the models constructed for algae cultivation and processing are described here. For parameters with sufficient data, we fit normal or lognormal distributions. For parameters with less data we fit triangular distributions, or uniform distributions when just a few data points were available.

2.1.1 Cultivation

Data for the green algae *Desmodesmus sp.,* which was grown at large scale under high-nitrogen conditions [1] were used to calculate productivity and lipid content. Specifically, we extended the calculations of Huntley et al. to estimate 95 percent prediction intervals for productivity and lipid content, in addition to the average values already reported [1]. Model fitting was conducted with the software package R 3.1.2 [15].

For productivity, the data presented in Figures 7(A), 9(A), and B-2 of Huntley et al. were fit to the linear models shown in Figure S1 a, b and c, and d, respectively. Assuming an initial total nitrogen concentration of 4.8 gm^{-2} (high-nitrogen case), and a particulate organic nitrogen concentration of 1.4 gm^{-2} on Day 1 (am), productivity (mean ± standard deviation, of 23 ± 4.8 $gm^{-2}day^{-1}$, assuming a normal distribution) was calculated using Figure S1 as described in Huntley et al. Similarly, for lipid content, the data presented in Figure 10 of Huntley et al. (*Desmodesmus*, Day 2), was fit to a linear model (Figure S2) to calculate lipid produced at the end of a two-day growth cycle. Lipid (gm^{-2}) was calculated for N = 4.2 gm^{2}, and the resulting value was divided by the DW of algae at the same nitrogen loading (Huntley et al. 2015). The resulting range of values for lipid content had a mean ± standard deviation of 0.37±0.07, and a normal distribution.

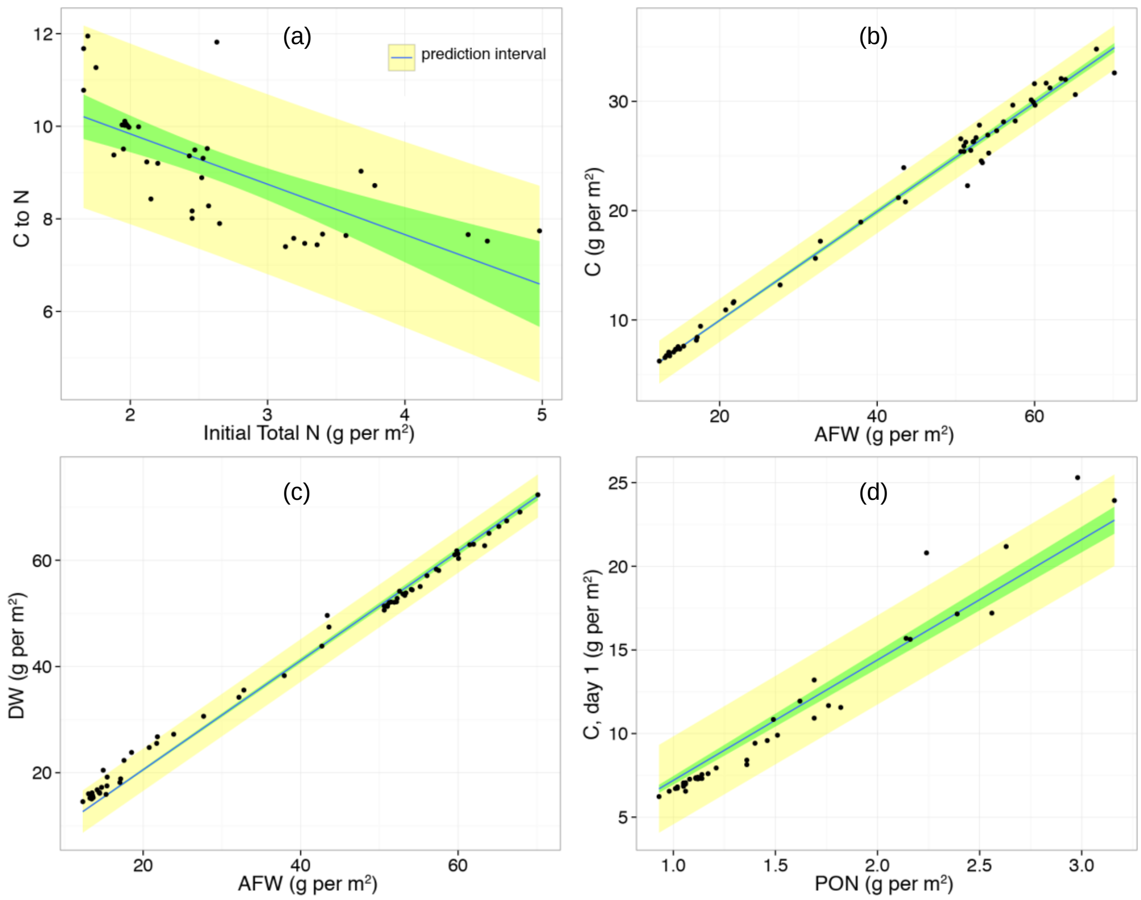

Figure S1. Linear fits (blue line) with 95 percent prediction intervals (yellow ribbon) for data (Huntley et al., 2015 [1)] used to calculate productivity of algae (gm^{-2}day^{-1}): (a) Ratio of particulate organic carbon (C) to nitrogen (N) versus initial total nitrogen in pond (N, gm^{-2}); (b) C (gm^{-2}) versus ash free weight of algae (AFW, gm^{-2}); (c) Dry weight of algae (DW, gm^{-2}) versus AFW (gm^{-2}); and (d) C, day 1 (gm^{-2}) versus particulate organic nitrogen (PON, gm^{-2}).

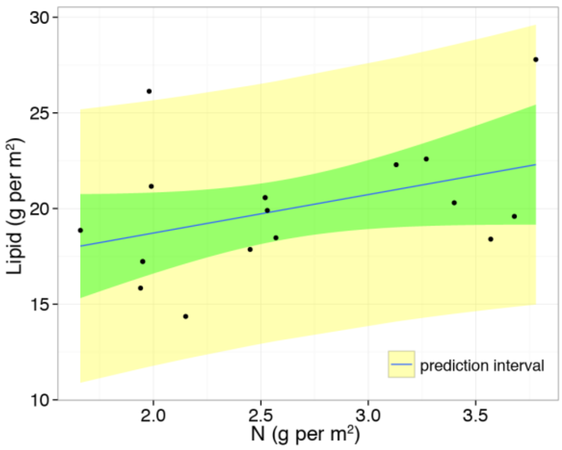

Figure S2. Linear fit (blue line) with 95 percent prediction interval (yellow ribbon) for data (Huntley et al., 2015 [1]) used to calculate lipid content of algae (g lipid/g DW): Lipid (gm²) versus initial nitrogen (gm²).

Table S9: distributions and associated parameters used to characterize the uncertainty associated with the foreground model parameters of the algae cultivation.

Model parameter	Distr. law	mode	min	max	mu	sigma
biomass productivity [g/m2/day]	normal				23	4.475
lipid fraction [-]	normal				0.37	0.07
stoichiometric CO2 requirement [g/g]	triangular	1.776	1.23	1.88		
efficiency of CO2 intake in ponds [-]	triangular	0.788	0.7	0.95		
capacity factor (valid also for processing) [-]	triangular	0.9	0.8	0.98		
electricity for dewatering [kWh/m3]	triangular	0.3	0.175			

For all the other cultivation parameters, although the design is based on the data of Beal et al [2], no data were available for the uncertainty ranges. Therefore, these have been approximated using the data presented in Sills et al [11], which modeled a similar cultivation facility (Table S9).

2.1.2 Processing

Table S10: distributions and associated parameters used to characterize the uncertainty associated with the foreground model parameters of the two pathways for algae processing.

Model parameter	Distr. law	mode	min	max	mu	sigma
Fuel only route (HTL)						
biocrude yield in HTL [-]	triangular	0.5	0.35	0.65		
specific heat required for HTL [MJ/kg algae]	lognormal				-0.86	0.18
specific elec. required for HTL [MJ/kg algae]	lognormal				-2.45	0.18
conversion yield to syngas in CHG [-]	uniform		0.55	0.69		
methane fraction of syngas in CHG [-]	uniform		0.52	0.59		
pressure of CHG [bar]	uniform		201	211		
Fuel and feed route (wet extraction of bio-oil)						
oil extraction efficiency [-]	uniform		0.7	0.9		
specific heat required for extraction [MJ/kg algae]	lognormal				-1.06	0.18
specific elec. required	lognormal				-1.13	0.18

for extraction [MJ/kg algae]						
heptane loss for extraction [-/g algae]	lognormal				-10.38	0.18

Values for the biocrude yield from HTL were taken from Frank et al [16], which reported experimental results for reactions at several temperatures and with several algae strains. Values for the specific heat and electricity requirements have been taken from Sills et al [11], but the uncertainty range was adapted to represent a more mature technology, which is the goal of the present study. Thus, the values that represent very high consumptions of heat and electricity have been removed, since they are not likely to occur with a commercial technology but only with an experimental setup.

Data for the conversion yield of biomass feed to syngas in catalytic hydrothermal gasification (CHG), as well as the methane fraction in syngas and the process operating pressure have been taken from Elliot et al [5] for the pilot-scale experiments conducted with algae. Since there were too few replicates available to fit a statistical distribution, a uniform distribution has been used.

For the fuel and feed pathway, a uniform distribution was used, based on the range provided in the sensitivity analysis of Beal et al [2] for the oil extraction efficiency. Modes for the electricity, heat and solvent consumption have also been taken from Beal et al [2], and their associated uncertainty ranges have been estimated using data of Sills et al [11].

2.2 Background LCI uncertainty

Uncertainties of off-site emissions in the life cycle inventory over the supply chain of materials, energy and waste disposal are also accounted for in the uncertainty model and in the Monte Carlo simulations. For that purpose, Monte Carlo simulations were run in the software SimaPro 8 [17] coupled with the ecoinvent v3.1 [10] database to simulate uncertainties associated with the life cycle inventories and to aggregate them in the four chosen final indicators: climate change, ecosystem quality, human health, and depletion of non-renewable resources. Then, using Matlab [18], a lognormal distribution was fit to the 1000 results from Monte Carlo simulations run within SimaPro. The parameters of the lognormal distribution associated with each equivalence of the LCI database ecoinvent v3.1 [10] have then been provided as input parameters for the Monte Carlo simulation of uncertainties in the Matlab computational framework presented here. Uncertainty parameters for the equivalences of the life cycle inventory are shown in Table S11 below.

Table S11: parameters of the lognormal distribution for background life cycle inventory data. The unit of the ecoinvent equivalence is given, as well as the location for which the equivalence is valid (GLO – Global; RoW – Rest of the World without Europe; US – USA; TRE – Texas).

ecoinvent equivalence	Impact category	Mu	Sigma
ammonia, liquid {RoW} - ammonia production, steam reforming, liquid [kg]	climate change	-8.63	0.192
	ecosystem quality	-11.5	0.226
	human health	-8.45	0.226
	resources	-8.28	0.176
electricity, medium voltage {TRE} – electricity voltage transformation from high to medium voltage [MJ]	climate change	-10.8	0.054
	ecosystem quality	-13.4	0.312
	human health	-10.6	0.312
	resources	-10.7	0.115

extrusion, plastic pipes {RoW} [kg]	climate change	-9.87	0.086
	ecosystem quality	-12.0	0.112
	human health	-9.41	0.112
	resources	-10.0	0.093
heat, district or industrial, natural gas {RoW} – heat production, natural gas, at boiler modulating >100kW [MJ]	climate change	-12.0	0.190
	ecosystem quality	-16.1	0.293
	human health	-12.0	0.293
	resources	-11.8	0.193
heptane {RoW} – molecular sieve separation of naphtha [kg]	climate change	-10.3	0.131
	ecosystem quality	-12.2	0.247
	human health	-10.1	0.212
	resources	-8.78	0.247
maize grain {US} [kg]	climate change	-9.97	0.104
	ecosystem quality	-10.0	0.116
	human health	-9.62	0.116
	resources	-10.3	0.116
methanol factory {GLO} [unit]	climate change	8.09	0.141
	ecosystem quality	8.58	0.181
	human health	9.44	0.181
	resources	8.02	0.141
low density polyethylene {RoW} [kg]	climate change	-8.25	0.188
	ecosystem quality	-10.5	0.212
	human health	-8.27	0.181
	resources	-7.43	0.212

petrol, low-sulfur {RoW} [kg]	climate change	-9.43	0.127
	ecosystem quality	-11.1	0.279
	human health	-8.76	0.279
	resources	-7.85	0.221
phosphate fertilizer, as P2O5 {RoW} – diammonium phosphate production [kg]	climate change	-8.75	0.181
	ecosystem quality	-8.64	0.227
	human health	-7.94	0.227
	resources	-8.70	0.227
polyvinylchloride, bulk polymerized {RoW} [kg]	climate change	-8.51	0.124
	ecosystem quality	-11.9	0.134
	human health	-9.17	0.134
	resources	-7.81	0.125
soybean meal {US} [kg]	climate change	-9.12	0.119
	ecosystem quality	-10.1	0.119
	human health	-9.97	0.119
	resources	-10.6	0.119
transport, freight, lorry 16-32 metric ton, EURO3 {RoW} [tkm]	climate change	-10.9	0.097
	ecosystem quality	-10.9	0.234
	human health	-12.1	0.179
	resources	-10.8	0.234
waste polyethylene/polypropylene product {RoW} – treatment of, collection for final disposal [kg]	climate change	-8.12	0.218
	ecosystem quality	-13.4	0.407
	human health	-10.0	0.407
	resources	-12.2	0.299

waste polyvinylchloride product {RoW}, treatment of, collection for final disposal [kg]	climate change	-8.37	0.207
	ecosystem quality	-10.5	0.265
	human health	-8.76	0.262
	resources	-9.60	0.265

2.3 Background economic uncertainty

Since for economics there is no equivalent of a LCI database with harmonized assumptions, data to characterize background uncertainty related to the model economic parameters were collected from literature sources and fit to probability distribution functions to generate uncertainty ranges. When enough data were available, normal or lognormal distributions were fit to the economic parameters. When insufficient information was available, a triangular or uniform distribution was used based on the available information. A summary of economic parameters and their associated probability distribution functions are described in Table S12 below.

Table S12: probability distribution functions and associated parameters used to characterize the uncertainty associated with the background parameters of the TEA model.

Economic parameter	Distr. law	mode	min	max	mu	sigma
ammonia price [$/MT]	normal				802	76
DAP price [$/MT]	normal				623	60
maintenance factor [-]	triangular	0.035	0	0.08		
electricity price [$/kWh]	lognormal				-2.65	0.26
natural gas price [$/kWh]	lognormal				-3.87	0.32
discount rate [-]	triangular	0.1	0.055	0.105		
tax rate [-]	triangular	0.2	0	0.4		

interest rate [-]	triangular	0.08	0.05	0.09		
error on investment estimate [-]	uniform		-0.2	0.3		
animal feed price [$/MT]	normal				587	47
equity [-]	triangular	0.4	0	1		
loan term [yr]	triangular	10	5	20		
fishmeal price [$/MT]	lognormal				7.44	0.14

Data for fertilizer prices, ammonia and diammonium phosphate, were taken from the National Agricultural Statistics Services online database of the US Department of Agriculture [19]. The electricity and natural gas data were taken from the online database of the US Energy Information Administration [20]. For lipid-extracted algae sold as animal feed, soybean meal price was assumed to be an equivalent, and data from the Food and Agriculture Organization was used [21]. Data for fishmeal prices, used for the fish feed scenarios were taken from the online data of the commodity market survey [22]. All economic data were taken from a period not prior to 2010 until 2015, when most up-to-date data were available.

The distributions of TEA parameters were estimated using data of several previous published TEA studies for algal biofuels or similar biorefinery processes. These data are compiled in Table S13 below. Since there was not enough data to fit normal or lognormal probability distribution functions, and that the boundaries of these parameters are fixed, a triangular distribution has been used, following the approach presented in Sills et al [11].

Table S13: summary of literature data for calculating the probability distribution functions associated with the TEA model parameters.

Study	capacity factor [-]	cultivation maintenance [-]	equipment maintenance [-]	discount rate [-]	tax rate [-]	interest rate [-]	equity [-]	loan term [yr]
Beal et al [2]	0.95	0.02	0.03	0.1	0.2	0.08	0.4	10
Davis et al [23]	N.A.	0.035	0.035	0.1	0.35	0.08	0.4	10
Lundquist et al [24]	N.A.	0.02	0.02	N.A.	0.0875	0.05	0	30
Amer et al [25]	0.91	0.01	0.05	N.A.	N.A.	0.06	0	15
Delrue et al [26]	N.A.	0.06	0.06	0.08	N.A.	N.A.	N.A.	20
Resureccion et al [27]	N.A.	N.A.	N.A.	0.06	0.2	N.A.	N.A.	N.A
Richardson et al [28]	N.A.	0.02	0.02	0.1	0.15	0.08	0.4	10
Slade and Bauen [29]	0.82/0.98	0.04	0.04	N.A.	0.16	N.A.	N.A.	N.A.
Zhu et al [30]	0.9	0.04	0.04	0.1	N.A.	N.A.	1	N.A.
Vlysidis et al [31]	N.A.	0.07	0.07	N.A.	0	0.07	N.A.	N.A.
Sun et al [32]	0.9	N.A.	N.A.	0.1	0.35	N.A.	N.A,	5/8/10/15/20

The TEA model corresponds to a Class 3 estimate of the Association for the Advancement of Cost Estimating (AACE). According to Lundquist et al [24], the error on the investment cost estimate for such an estimate should be between -20% and +30%. In the absence of any other data, a uniform probability distribution function for this parameter was assumed with this range.

2.4 Monte-Carlo simulations

The number of iterations in a Monte-Carlo simulation was determined by repeating the Monte-Carlo simulation with a fixed number of iterations (up to 10 000), and by verifying that the results stayed within a certain precision range. For the minimum selling price of biocrude, we selected a precision of <0.1 USD for the median, the quartiles, and the 5% and 95% quantiles, which are the values that we used to report graphically our results. 1000 iterations were determined to be a sufficient number of iterations following that methodology.

3 Supplementary results

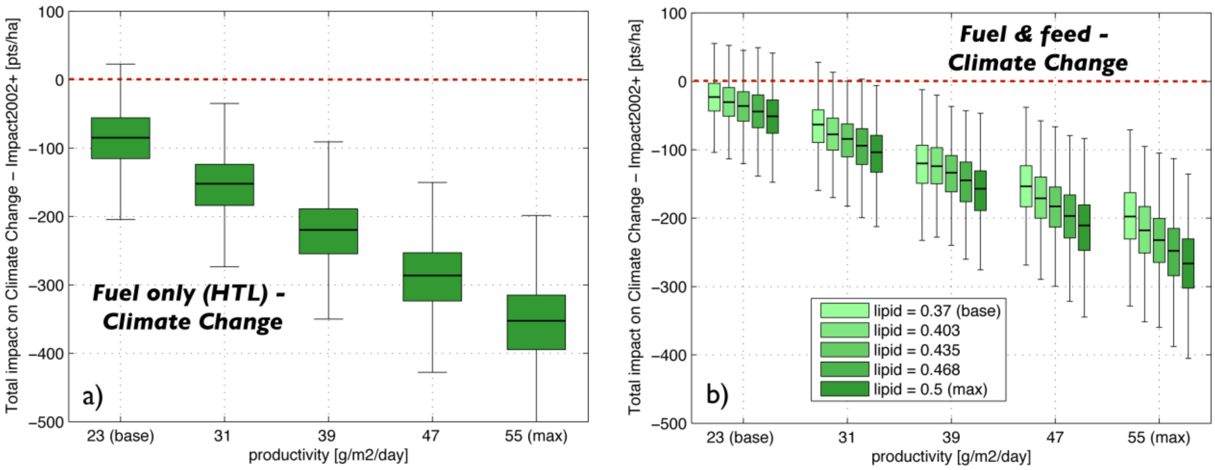

Figure S3: Effect of productivity and lipid content improvement on climate change indicator. Center lines represent median values, edges of boxes represent 25th and 75th percentiles, and limiting bars represent 5th and 95th percentiles of the distributions resulting from 1 000 Monte Carlo simulations.

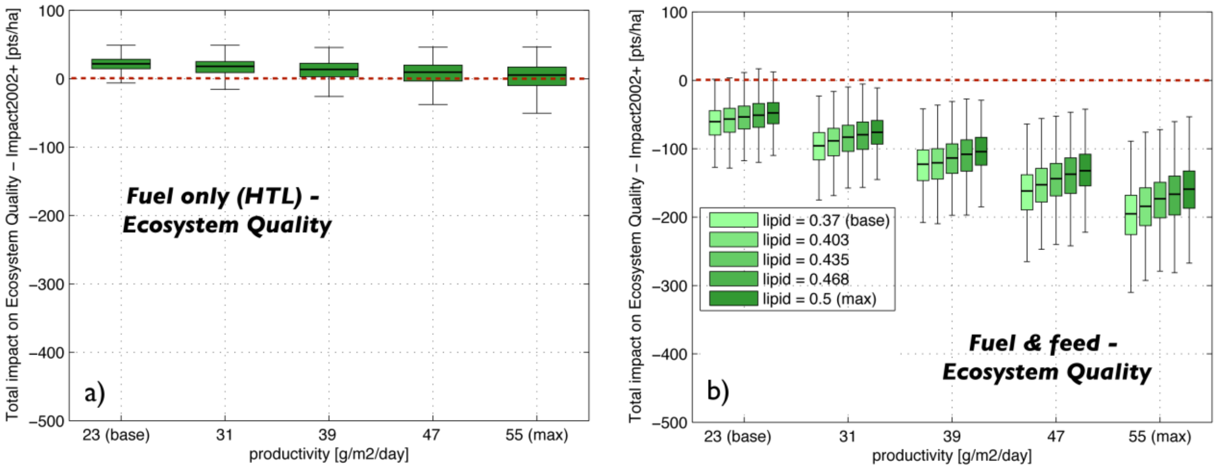

Figure S4: Effect of productivity and lipid content improvement on ecosystem quality indicator. Center lines represent median values, edges of boxes represent 25th and 75th percentiles, and limiting bars represent 5th and 95th percentiles of the distributions resulting from 1 000 Monte Carlo simulations.

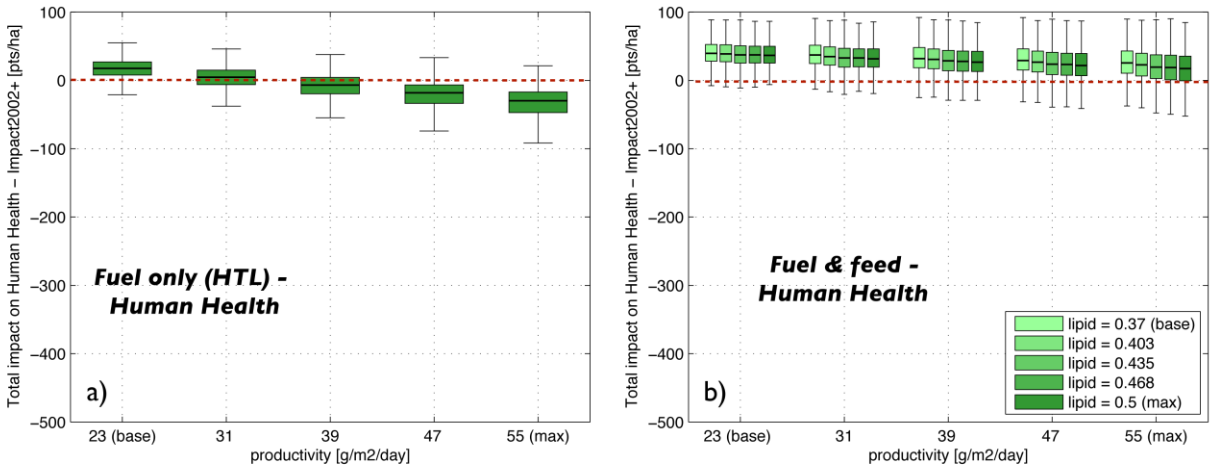

Figure S5: Effect of productivity and lipid content improvement on human health indicator. Center lines represent median values, edges of boxes represent 25th and 75th percentiles, and limiting bars represent 5th and 95th percentiles of the distributions resulting from 1 000 Monte Carlo simulations.

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