Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supplementary material to "*Evaluation of the potential use of e-fuels in the European aviation sector: A comprehensive economic and environmental assessment including externalities.*"

Diego Freire Ordóñez,[ab] Thorsteinn Halfdanarson,[c] Caroline Ganzer,[ac] Nilay Shah,[a] Niall Mac Dowell,[ac] and Gonzalo Guillén-Gosálbez*[d]

[a.] *The Sargent Centre for Process Systems Engineering, Imperial College London, UK.*
[b.] *Institute for Applied Sustainability Research, Quito, Ecuador*
[c.] *Centre for Environmental Policy, Imperial College London, UK*
[d.] *Institute for Chemical and Bioengineering, ETH Zürich, Switzerland. E-mail:* *gonzalo.guillen.gosalbez@chem.ethz.ch*

Contents

This document is divided into four appendixes, including critical data used in the calculations and some intermediate results as explained hereafter. In Appendix A, the design parameters of the Fischer-Tropsh (*FT*) and hydrocracking (*HC*) processes are given, along with the simulation results of a basic characterisation of e-jet fuel, including the weight-based distribution, density, net heating value (*NHV*), boiling point, flash point and freezing point, compared with standard values for conventional jet fuel A-1. Appendix B includes the life-cycle inventory (*LCI*) utilised for the *LCA* of green H_2 and e-jet fuels, the combustion factors for the fuels and additional information regarding the particular processes not included in Ecoinvent 3.5. Appendix C provides the information required for the economic assessment of green H_2 and e-jet fuels, *i.e.*, economic parameters and assumptions, equipment cost data, and costs of raw materials, utilities and by-products. Finally, in Appendix D, the *ReCiPe* 2016 *LCA* results at the midpoint level of the studied e-jet fuels are provided.

Abbreviations

α	Chain growth probability	ACC	Annualised capital cost
AP	Annual production	APOS	Allocation at the point of substitution
ASF	Anderson-Schulz-Flory	BAU	Business as usual
BECCS	Bioenergy with carbon capture and storage/sequestration	BOP	Balance of plant
		CAPEX	Capital expenditure
CCU	Carbon capture and utilisation	CEPCI	Chemical engineering plant cost index
CF	Capacity factor	D	Scaling factor
DE	Germany	EQ	Ecosystems quality
ES	Spain	FCI	Fixed capital investment
FR	France	FT	Fischer-Tropsch
GB	United Kingdom	GWP	Global warming potential
HC	Hydrocracking	HH	Human health
HI	Heat integration	HRAT	Heat recovery approach temperature
i	Interest rate	IT	Italy
LCA	Life cycle assessment	MCC	Mortality cost of carbon emissions
NHV	Net heating value	NPC	Net production cost
OPEX	Operational expenditure	PC	Purchased cost of equipment
PEM	Polymer electrolyte membrane	PEMEL	PEM electrolyser
PR-BM	Peng-Robinson equation of state with Boston-Mathias alpha function	PtF	Power-to-fuels
		PtL	Power-to-liquids
PV	Photovoltaic	RS	Resource scarcity
rWGS	Reverse water-gas shift	S	Actual size of equipment
SCC	Social cost of carbon emissions	t	Plant economic life
TCI	Total capital investment	TOC	Total operating cost
TRL	Technology readiness level	WC	Working capital
y	Year		

Appendix A e-fuel composition and main properties

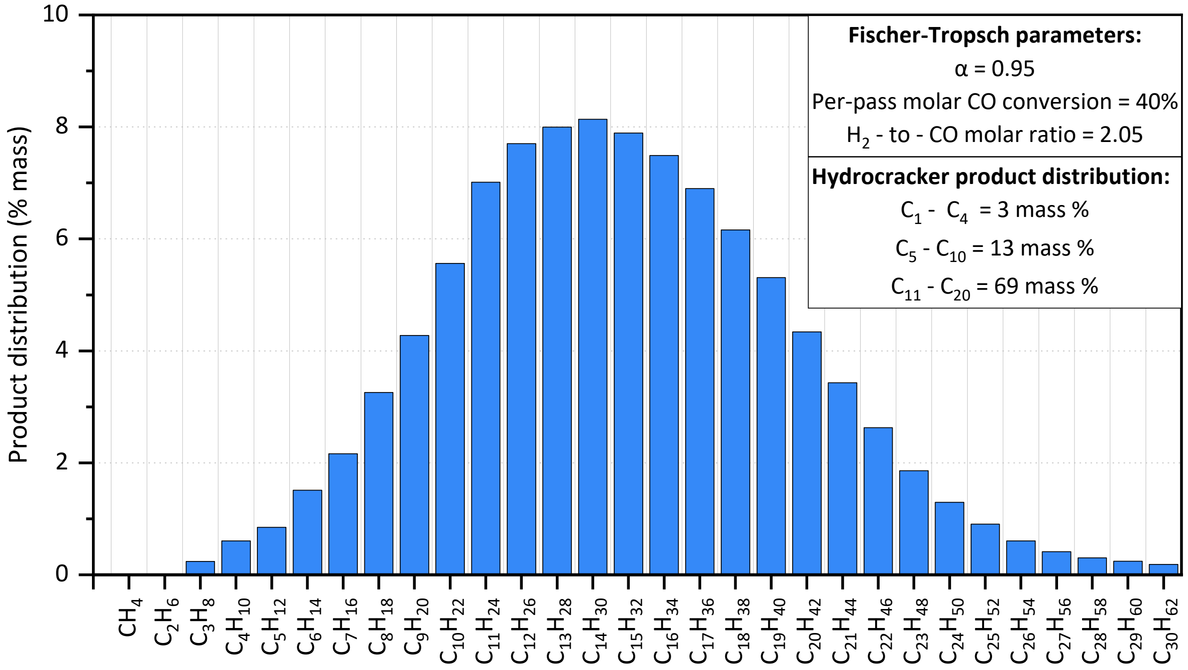

Fig. A-1: Mass-based product distribution.

Table A-1. Properties of conventional jet fuel A-1 and e-jet fuel.

Properties	**e-jet fuel (from simulation)**	**Jet fuel A-1 (according to *ASTM* D7566)**
Density @ 15°C (kg/m^3)	758.1	775-840
NHV (MJ/kg)	43.73	> 42.8
Average boiling point (°C)	229.35	150 to 300
Flash point (°C)	39.12	> 38
Freezing point (°C)	-51.6	Max. -47

Appendix B *LCA* inventories

Table B-1. Inventory data of the foreground system for the production of e-jet fuel after heat integration.

Products				
Outputs to technosphere: Products and co-products	**Amount**	**Unit**		
e-jet fuel	5.20×10^{8}	kg		
Inputs				
Inputs from nature	**Amount**	**Unit**	**Distribution**	**2SD**
Air (for burner)	1.00×10^{9}	kg	Lognormal	1.09
Inputs from technosphere: materials/fuels				
Water, deionised, from tap water	6.01×10^{8}	kg	Lognormal	1.09
H_2 from electrolysis including storage (see Table B-3)	2.51×10^{8}	kg	Lognormal	1.09
Captured CO_2 (see Table B-4)	1.95×10^{9}	kg	Lognormal	1.09
rWGS: nickel-based catalyst [1,2]	9.68×10^{2}	kg	Lognormal	1.09
FT: cobalt-based catalyst [3,4]	7.34×10^{2}	kg	Lognormal	1.09
HC: platinum-based catalyst [5,6]	1.15×10^{3}	kg	Lognormal	1.09
Steel, chromium steel 18/8, with 70% end-life recycling[7]	4.04×10^{6}	kg	Lognormal	1.09
Inputs from technosphere: electricity/heat				
Electricity, high voltage, market for	1.01×10^{6}	MWh	Lognormal	1.09
Cooling water [8]	2.03×10^{6}	MWh	Lognormal	1.09
Outputs				
Emissions to air				
Water	1.09×10^{8}	kg	Lognormal	1.51
Hydrogen	9.43×10^{1}	kg	Lognormal	1.51
Carbon monoxide	4.23×10^{3}	kg	Lognormal	5.01
Oxygen	3.88×10^{7}	kg	Lognormal	1.51
Carbon dioxide, process	3.50×10^{8}	kg	Lognormal	1.09
Outputs to technosphere: Waste treatment				
Wastewater, market for	2.42×10^{6}	m^3	Lognormal	1.09
Catalysts, used	2.35×10^{7}	kg	Lognormal	1.09

Table B-2. Emission factors for the combustion of e-jet fuel and fossil jet fuel.

	Feedstock/Product	Fossil fuel emissions[9]	e-jet fuel emissions*	Unit
CO_2	Product	3.16	3.09	kg CO_2/kg fuel
H_2O	Product	1.24	1.21	kg H_2O /kg fuel
NO_x	Product	1.00	0.98	kg NO_x /kg fuel
CO	Product	1.75	1.71	kg CO/kg fuel
Air (24 wt.% O_2)	Feedstock	14.17	13.84	kg air/kg fuel

* From the carbon balance of the components in the e-jet fuel product stream

Table B-3. Inventory data of the foreground system per kilogram of H_2 (30 bar) based on the results of the *gAWE* model for each location.

Products	***GB***	***DE***	***FR***	***ES***	***IT***	
Outputs to technosphere: Products and co-products	**Amount**	**Amount**	**Amount**	**Amount**	**Amount**	**Unit**
H_2 from electrolysis	1	1	1	1	1	kg
O_2 from electrolysis	7.94	7.94	7.94	7.94	7.94	kg
Inputs						
Inputs from technosphere: materials/fuels						
Water, deionised, from tap water	8.94	8.94	8.94	8.94	8.94	kg
H_2 storage required (Type I tanks[10,11] or salt caverns[12,+])	0.0128	0.0265	0.01429	0.0238	0.0207	kg
Inputs from technosphere: electricity/heat						
Electricity, photovoltaic, open ground installation*	9.41	25.22	20.21	14.75	30.12	kWh
Electricity, wind, >3MW turbine*	46.89	31.08	36.09	41.55	26.18	kWh

[+] *Here, only the electricity consumption for compression and drying is considered

* We assume a current energy demand for water electrolysis of 56.3 kWh/kg H_2 (59% efficiency) [13,14]

Table B-4. Inventory data of the foreground system per kilogram of captured CO_2 (1 bar) for each source.

Products	***C-PP***[15]	***NG-PP***[16]	***DAC-HT***[17]	***DAC-LT***[18]	
Outputs to technosphere: Products and co-products	**Amount**	**Amount**	**Amount**	**Amount**	**Unit**
Captured CO_2	1	1	1	1	kg
Outputs to technosphere: Avoided products					
Electricity, high voltage, production	0.88	3.29			kWh
Inputs					
Inputs from nature					
Air		20193.55			g
Cooling water, unspecified natural origin		1451.61			g
Inputs from technosphere: materials/fuels					
Light fuel oil, market for	6.22				g
Natural gas liquids, market for	0.82	478.45	125.00		g
Hard coal, market for	521.09				g
Monoethanolamine, market for	1.54	8.77			g
Neutralising agent, sodium hydroxide-equivalent, market for	0.12				g
Ammonia, liquid, market for	1.15				g
Limestone, crushed, washed, market for	43.12				g
Tap water, market for		1064.52	3105.26		g
Spent catalyst, market for		0.0029			g
Calcium carbonate, precipitated, market for			19.88		g
Adsorbent (Amine on alumina)[18]				7.5	g
Inputs from technosphere: electricity/heat					
Electricity, high voltage, production mix			0.2340	0.7	kWh
Heat, district or industrial, municipal waste incinerat., market for				11.9	MJ
Outputs					
Emissions to air					
Particulates, < 2.5 um	0.11				g
Ammonia	0.27				g
Monoethanolamine	0.09	3.52			g
Nitrogen oxides	1.06	1.58			g
Sulfur dioxide	0.07				g
Carbon dioxide, fossil	52.44	328.65	-1000	-1000	g
Water		1645.16			g
Outputs to technosphere: Waste treatment					
Hazardous waste, treatment, underground deposit	2.27				g
Municipal solid waste, treatment, open dump	1.81				g
Wastewater, market for		0.0016			m^3
Spent catalyst, treatment		0.0029			g

Appendix C Data for the economic evaluation

Table C-1. Economic parameters and assumptions.

Parameter	Value				
Location (latitude, longitude)	*GB* (56, -6)	*DE* (48, 12)	*FR* (48, 0)	*ES* (40, -6)	*IT* (40, 18)
Base year	2018	2018	2018	2018	2018
Plant economic life (y)[19–21]	20	20	20	20	20
Plant availability (h/y)[22]	8260	8260	8260	8260	8260
Interest rate (%)[23]	8.30%	6.80%	7.20%	8.20%	7.20%

Table C-2. H_2 production plant: Cost input data.

Equipment	Sizing based on:	USD_{2018} per size unit	Reference
Photovoltaic (*PV*) solar panels	1 kW installed capacity	1210	[24]
Wind turbines onshore	1 kW installed capacity	1497	[24]
Wind turbines offshore	1 kW installed capacity	4353	[24]
PEMEL	1 kg/h H_2	56300	[14]
Electrical energy storage: Lithium-ion batteries	1 kWh electricity	418	[25]
H_2 storage: Type I tanks	1 kg H_2	755	[11]
H_2 storage: Salt caverns	1 kg H_2	215	[26]

Table C-3. Fuel production plant: *CAPEX* of special equipment cost data.

Equipment	PC_{ref}	Unit	S_{ref}	Design variable	Unit	D	Reference year	Reference
Burner	2.62	MUSD	20.00	Heat duty	MW	0.83	2014	[22]
Hydrocracker	10.36	MUSD	1.13	Feed rate	kg/s	0.70	2014	[22]
rWGS reactor	3.19	MUSD	2556.00	Flowrate	t/day	0.65	2014	[22]
FT reactor	10.50	MUSD	2.52	Feed rate	Mscf/h	0.72	2003	[27]

Table C-4. Fuel processing plant: *OPEX* data at 2018 prices.

Raw material/Utility	Value for 2018	Unit	Reference
CO_2 from *C-PP*	0.0043	USD_{2018} /kg	[28]
CO_2 from *NG-PP*	0.064	USD_{2018} /kg	[28]
CO_2 from *DAC-HT*	0.16	USD_{2018} /kg	[17]
CO_2 from *DAC-LT*	1.10	USD_{2018} /kg	[29]
Grid electricity (Non-household consumers) (*GB*)	158.67	USD_{2018} /MWh	[30]
Grid electricity (Non-household consumers) (*DE*)	127.68	USD_{2018} /MWh	[30]
Grid electricity (Non-household consumers) (*FR*)	62.18	USD_{2018} /MWh	[30]
Grid electricity (Non-household consumers) (*ES*)	103.16	USD_{2018} /MWh	[30]

Grid electricity (Non-household consumers) (*IT*)	110.72	USD_{2018} /MWh	[30]
Process H_2O	1.09	USD_{2018} /t	[19]
Cooling water	1.35	USD_{2018} /MWh	[31]
Wastewater disposal	0.44	USD_{2018}/t	[19]

Appendix D *LCA* results at midpoint level

Table D-1. e-jet fuel from CO_2 from coal-based power plants (*C-PP*).

		GB		*DE*		*FR*		*ES*		*IT*	
Impact category	*Unit*	*Tanks*	*Caverns*	*Tanks*	*Caverns*	*Tanks*	*Caverns*	*Tanks*	*Caverns*	*Tanks*	*Caverns*
Global warming	kg CO_2 eq	3.361	3.357	4.446	4.437	2.806	2.802	2.780	2.772	3.731	3.725
Stratospheric ozone depletion	mg CFC-11 eq	1.488	0.709	1.926	0.320	1.586	0.719	1.991	0.549	1.925	0.671
Ionising radiation	kBq Co-60 eq	0.992	0.459	1.532	0.435	1.885	1.293	1.440	0.454	1.133	0.275
Ozone formation, Human health	g NOx eq	5.864	4.775	12.083	9.838	4.399	3.187	0.217	-1.800	6.818	5.064
Fine particulate matter formation	g $PM_{2.5}$ eq	2.497	1.221	9.365	6.733	2.071	0.650	-0.756	-3.122	4.571	2.515
Ozone formation, Terrestrial ecosystems	g NO_x eq	6.476	4.902	13.312	10.069	5.105	3.354	1.248	-1.666	7.813	5.280
Terrestrial acidification	g SO_2 eq	2.551	1.985	18.432	17.265	0.270	-0.360	-9.511	-10.559	6.177	5.265
Freshwater eutrophication	g P eq	2.108	1.509	4.895	3.661	2.141	1.475	2.530	1.421	2.772	1.808
Marine eutrophication	g N eq	0.258	0.159	0.523	0.319	0.296	0.186	0.344	0.160	0.359	0.200
Terrestrial ecotoxicity	kg 1,4-DCB	33.511	25.618	60.430	44.160	41.791	33.006	41.302	26.682	51.056	38.348
Freshwater ecotoxicity	kg 1,4-DCB	1.012	0.952	1.169	1.045	0.968	0.902	1.024	0.913	0.941	0.844
Marine ecotoxicity	kg 1,4-DCB	1.265	1.181	1.492	1.319	1.220	1.127	1.289	1.133	1.199	1.063
Human carcinogenic toxicity	kg 1,4-DCB	0.147	0.183	0.298	0.373	0.192	0.232	0.110	0.177	0.203	0.262
Human non-carcinogenic toxicity	kg 1,4-DCB	8.383	6.300	13.386	9.093	8.794	6.476	9.975	6.117	10.207	6.854
Land use	m^2a crop eq	0.340	0.230	0.694	0.468	0.427	0.305	0.413	0.210	0.593	0.417
Mineral resource scarcity	g Cu eq	29.064	26.630	40.239	35.222	32.950	30.241	31.602	27.094	34.753	30.834
Fossil resource scarcity	kg oil eq	1.103	0.823	1.682	1.105	1.004	0.693	1.240	0.722	1.411	0.961
Water consumption	m^3	0.039	0.025	0.086	0.058	0.058	0.042	0.056	0.030	0.082	0.060

Table D-2. e-jet fuel from CO_2 from natural gas-based power plants (*NG-PP*).

		GB		*DE*		*FR*		*ES*		*IT*	
Impact category	*Unit*	*Tanks*	*Caverns*	*Tanks*	*Caverns*	*Tanks*	*Caverns*	*Tanks*	*Caverns*	*Tanks*	*Caverns*
Global warming	kg CO_2 eq	3.651	3.647	3.770	3.761	0.751	0.746	1.833	1.825	2.636	2.629
Stratospheric ozone depletion	mg CFC-11 eq	0.981	0.202	1.736	0.130	-0.356	-1.222	0.768	-0.674	0.775	-0.479
Ionising radiation	kBq Co-60 eq	1.000	0.468	1.552	0.454	1.902	1.309	1.449	0.462	1.150	0.293
Ozone formation, Human health	g NOx eq	5.009	3.920	5.996	3.751	1.717	0.505	4.412	2.395	4.695	2.942
Fine particulate matter formation	g $PM_{2.5}$ eq	6.020	4.744	7.745	5.113	4.977	3.556	7.005	4.640	6.918	4.862
Ozone formation, Terrestrial ecosystems	g NO_x eq	5.772	4.199	7.224	3.981	2.458	0.707	5.527	2.613	5.690	3.157
Terrestrial acidification	g SO_2 eq	12.239	11.673	12.446	11.279	7.769	7.139	11.739	10.690	11.695	10.783
Freshwater eutrophication	g P eq	2.235	1.637	4.812	3.578	2.113	1.447	2.579	1.470	2.737	1.773
Marine eutrophication	g N eq	0.381	0.282	0.637	0.433	0.407	0.297	0.457	0.274	0.472	0.313
Terrestrial ecotoxicity	kg 1,4-DCB	34.334	26.442	60.509	44.239	42.772	33.987	42.134	27.515	51.341	38.633
Freshwater ecotoxicity	kg 1,4-DCB	1.023	0.963	1.167	1.044	0.967	0.900	1.030	0.919	0.940	0.844
Marine ecotoxicity	kg 1,4-DCB	1.268	1.183	1.484	1.311	1.208	1.115	1.296	1.140	1.197	1.061
Human carcinogenic toxicity	kg 1,4-DCB	0.209	0.245	0.300	0.375	0.194	0.234	0.154	0.221	0.207	0.266
Human non-carcinogenic toxicity	kg 1,4-DCB	8.545	6.462	13.319	9.026	8.784	6.466	10.043	6.185	10.183	6.829
Land use	m^2a crop eq	0.323	0.214	0.673	0.447	0.406	0.284	0.393	0.190	0.572	0.396
Mineral resource scarcity	g Cu eq	30.165	27.731	40.769	35.752	32.925	30.217	31.281	26.773	35.119	31.201
Fossil resource scarcity	kg oil eq	0.662	0.382	0.826	0.249	-0.249	-0.561	0.143	-0.376	0.619	0.168
Water consumption	m^3	0.037	0.023	0.084	0.055	0.052	0.037	0.066	0.040	0.082	0.060

Table D-3. e-jet fuel from CO_2 from direct air capture based on a high temperature, liquid solvent system (*DAC-HT*).

		GB		*DE*		*FR*		*ES*		*IT*	
Impact category	*Unit*	*Tanks*	*Caverns*	*Tanks*	*Caverns*	*Tanks*	*Caverns*	*Tanks*	*Caverns*	*Tanks*	*Caverns*
Global warming	kg CO_2 eq	2.806	2.802	3.980	3.971	1.838	1.834	2.321	2.314	3.160	3.154
Stratospheric ozone depletion	mg CFC-11 eq	1.952	1.173	3.799	2.193	1.958	1.091	2.593	1.151	3.117	1.863
Ionising radiation	kBq Co-60 eq	1.162	0.630	1.659	0.561	2.423	1.831	1.615	0.628	1.156	0.298
Ozone formation, Human health	g NOx eq	7.588	6.499	9.605	7.360	5.730	4.518	8.628	6.610	8.937	7.184
Fine particulate matter formation	g $PM_{2.5}$ eq	6.329	5.052	8.538	5.906	5.436	4.015	7.871	5.506	8.037	5.981
Ozone formation, Terrestrial ecosystems	g NO_x eq	8.253	6.680	10.884	7.641	6.481	4.730	9.711	6.796	9.990	7.457
Terrestrial acidification	g SO_2 eq	13.299	12.733	15.417	14.250	9.265	8.635	13.878	12.829	15.449	14.537
Freshwater eutrophication	g P eq	2.367	1.768	5.650	4.416	2.107	1.441	2.713	1.605	2.844	1.880
Marine eutrophication	g N eq	0.264	0.165	0.567	0.363	0.289	0.179	0.341	0.158	0.355	0.196
Terrestrial ecotoxicity	kg 1,4-DCB	34.860	26.967	61.090	44.820	43.490	34.706	42.928	28.309	52.037	39.329
Freshwater ecotoxicity	kg 1,4-DCB	1.027	0.967	1.191	1.067	0.969	0.902	1.037	0.926	0.946	0.850
Marine ecotoxicity	kg 1,4-DCB	1.288	1.204	1.523	1.349	1.222	1.128	1.309	1.152	1.207	1.071
Human carcinogenic toxicity	kg 1,4-DCB	0.218	0.254	0.342	0.417	0.200	0.241	0.173	0.240	0.219	0.277
Human non-carcinogenic toxicity	kg 1,4-DCB	8.704	6.622	13.984	9.691	8.864	6.546	10.230	6.372	10.356	7.002
Land use	m^2a crop eq	0.356	0.246	0.689	0.463	0.410	0.288	0.404	0.201	0.589	0.412
Mineral resource scarcity	g Cu eq	30.209	27.776	41.543	36.526	34.367	31.659	32.942	28.434	36.181	32.263
Fossil resource scarcity	kg oil eq	1.385	1.105	1.896	1.319	1.115	0.803	1.454	0.936	1.636	1.185
Water consumption	m^3	0.057	0.043	0.106	0.077	0.077	0.061	0.075	0.049	0.106	0.084

Table D-4. e-jet fuel from CO_2 from direct air capture based on a low temperature, solid sorbent system (*DAC-LT*)

		GB		*DE*		*FR*		*ES*		*IT*	
Impact category	*Unit*	*Tanks*	*Caverns*	*Tanks*	*Caverns*	*Tanks*	*Caverns*	*Tanks*	*Caverns*	*Tanks*	*Caverns*
Global warming	kg CO_2 eq	3.954	3.950	5.495	5.487	2.978	2.973	4.011	4.004	5.296	5.290
Stratospheric ozone depletion	mg CFC-11 eq	3.681	2.902	6.091	4.485	5.674	4.807	4.250	2.808	5.481	4.227
Ionising radiation	kBq Co-60 eq	1.572	1.039	1.940	0.843	3.545	2.952	1.962	0.976	1.238	0.380
Ozone formation, Human health	g NOx eq	11.401	10.312	12.325	10.080	11.231	10.019	16.747	14.730	15.725	13.972
Fine particulate matter formation	g $PM_{2.5}$ eq	8.435	7.159	10.015	7.383	8.384	6.963	11.579	9.214	12.984	10.928
Ozone formation, Terrestrial ecosystems	g NO_x eq	12.081	10.508	13.624	10.381	12.012	10.261	17.862	14.948	16.833	14.300
Terrestrial acidification	g SO_2 eq	19.376	18.810	20.204	19.037	18.195	17.565	24.626	23.578	31.201	30.289
Freshwater eutrophication	g P eq	2.831	2.232	7.696	6.462	2.234	1.567	3.013	1.905	3.175	2.211
Marine eutrophication	g N eq	0.365	0.267	0.768	0.564	0.381	0.271	0.430	0.247	0.448	0.289
Terrestrial ecotoxicity	kg 1,4-DCB	37.484	29.591	65.701	49.431	48.821	40.037	47.145	32.525	58.360	45.652
Freshwater ecotoxicity	kg 1,4-DCB	1.055	0.995	1.276	1.152	0.983	0.916	1.055	0.943	0.969	0.872
Marine ecotoxicity	kg 1,4-DCB	1.334	1.250	1.642	1.468	1.245	1.151	1.336	1.180	1.242	1.107
Human carcinogenic toxicity	kg 1,4-DCB	0.281	0.317	0.474	0.549	0.238	0.278	0.220	0.288	0.267	0.326
Human non-carcinogenic toxicity	kg 1,4-DCB	9.694	7.611	16.599	12.305	9.425	7.107	10.867	7.009	11.145	7.792
Land use	m^2a crop eq	0.865	0.755	0.859	0.634	0.725	0.603	0.883	0.680	1.012	0.836
Mineral resource scarcity	g Cu eq	35.555	33.121	56.095	51.078	39.635	36.926	36.310	31.802	40.673	36.754
Fossil resource scarcity	kg oil eq	1.930	1.651	2.034	1.457	1.249	0.937	1.678	1.160	2.046	1.595
Water consumption	m^3	0.055	0.041	0.107	0.078	0.102	0.087	0.103	0.077	0.151	0.129

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