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Two-Step Production of a Furfural-Derived Biosolvent in a Single Reactor: an Economic and Life Cycle Assessment Study

C. Yezerguelian[b] and M. Pera-Titus[a*]

[a] Cardiff Catalysis Institute, School of Chemistry, Cardiff University, Cardiff CF10 3AT, UK

[b] Syensqo, Research & Innovation Centre of Lyon, 85 Avenue des Frères Perret, 69192 Saint Fons, France

[*] Corresponding author. Tel.: +86 (0) 472445368, Fax: +86 (0) 472445399, E-mail: peratitusm@cardiff.ac.uk

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ELECTRONIC SUPPORTING INFORMATION

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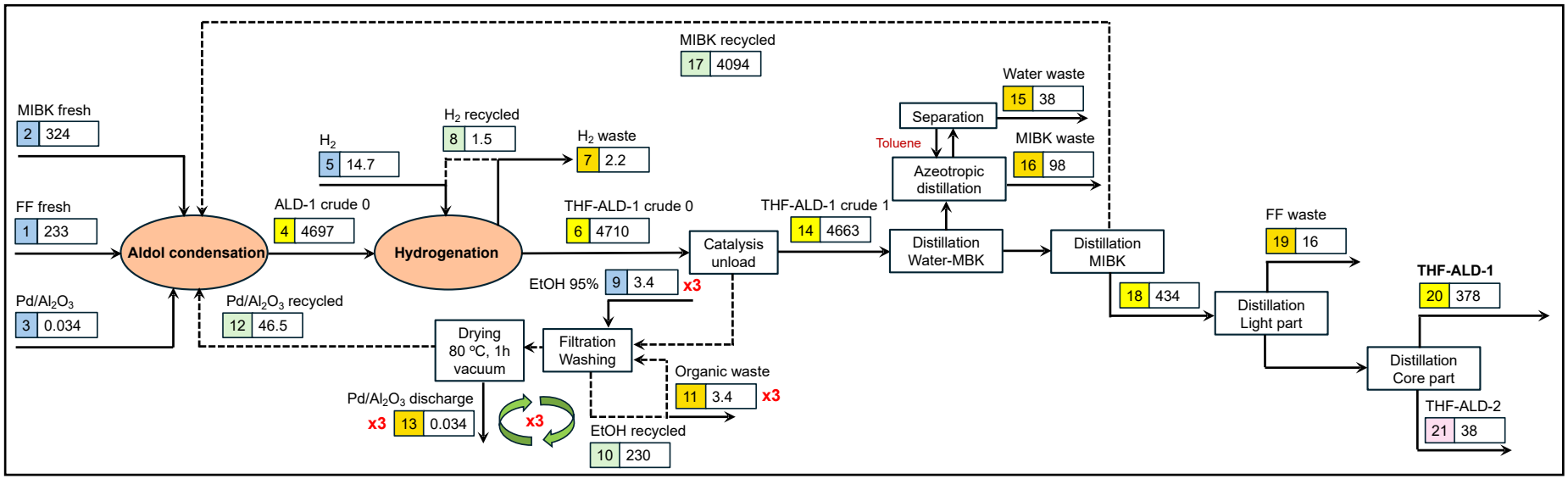

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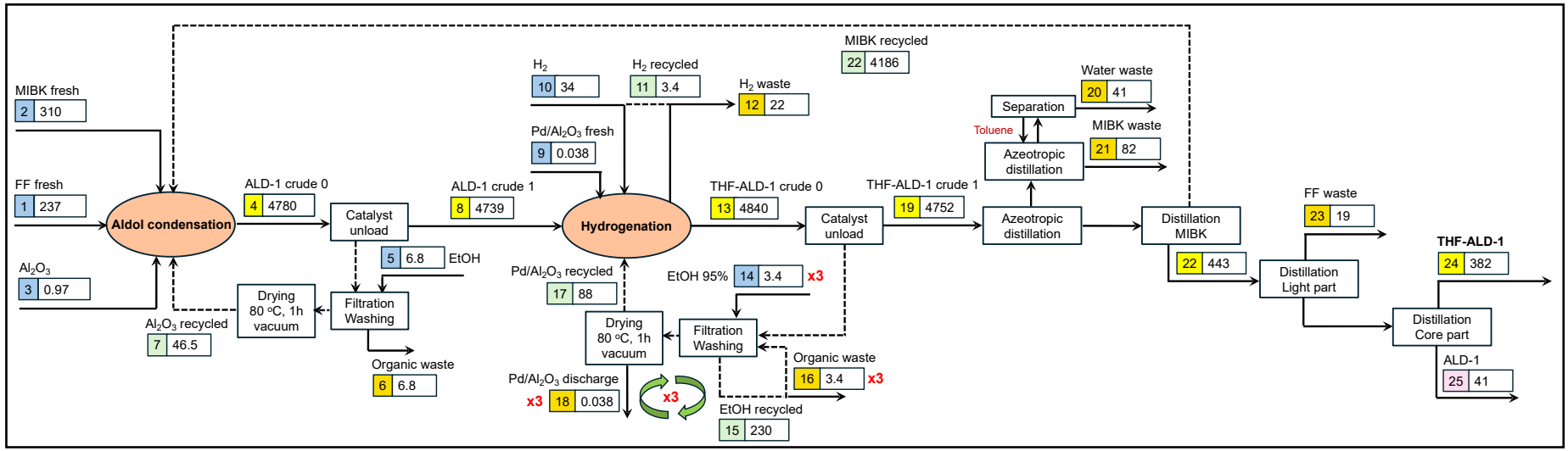
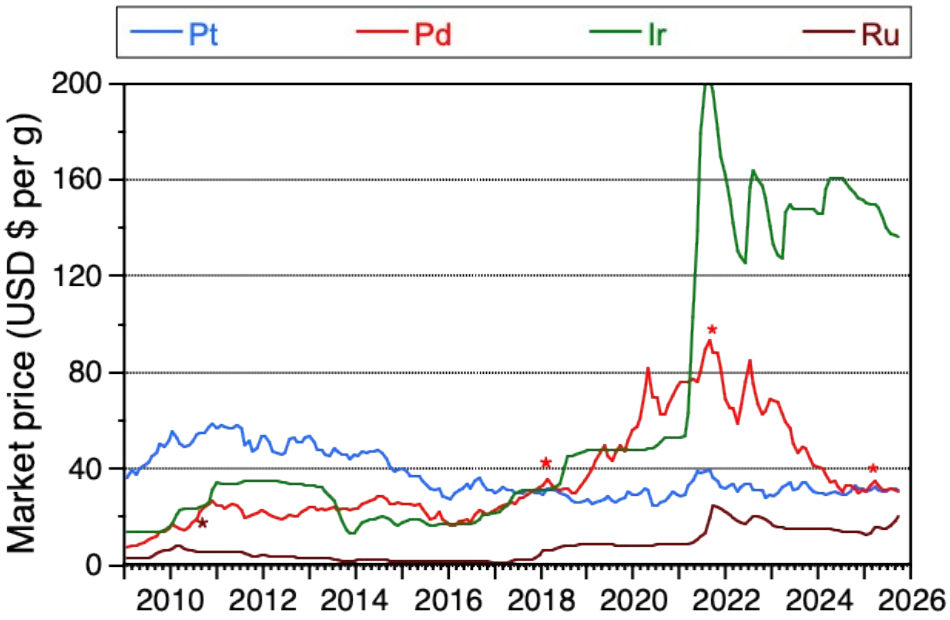


Fig S2. Flowsheet for two-reactor aldol condensation – hydrogenation process.



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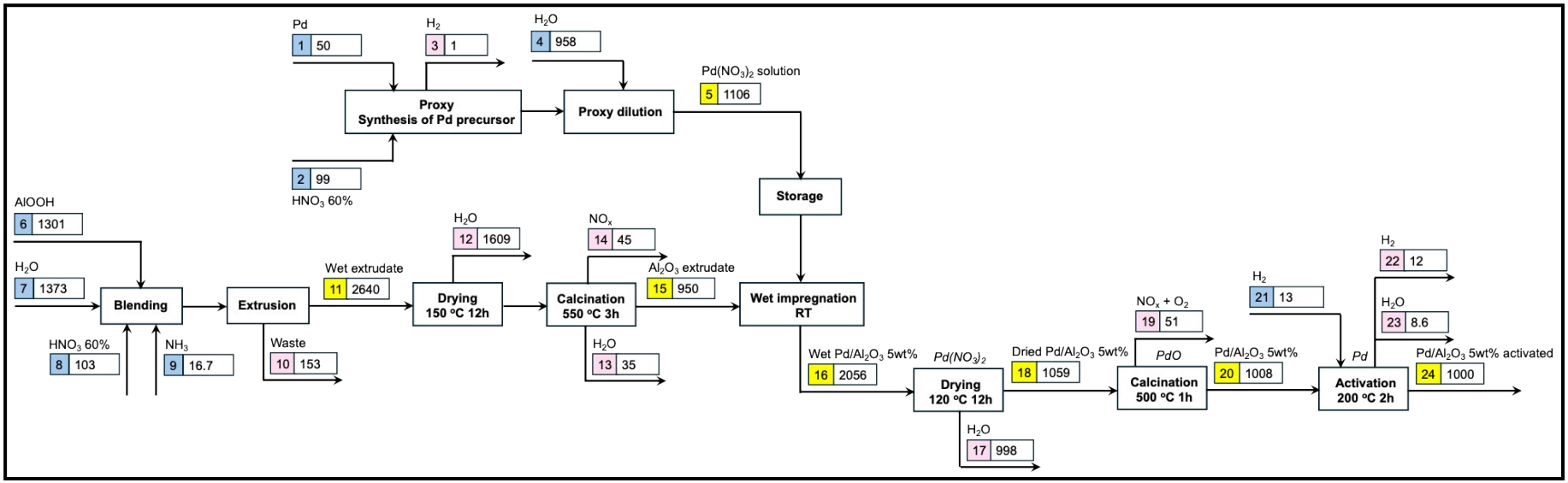


Fig S4. Flowsheet for the process for preparing Pd/Al_2O_3 catalyst.

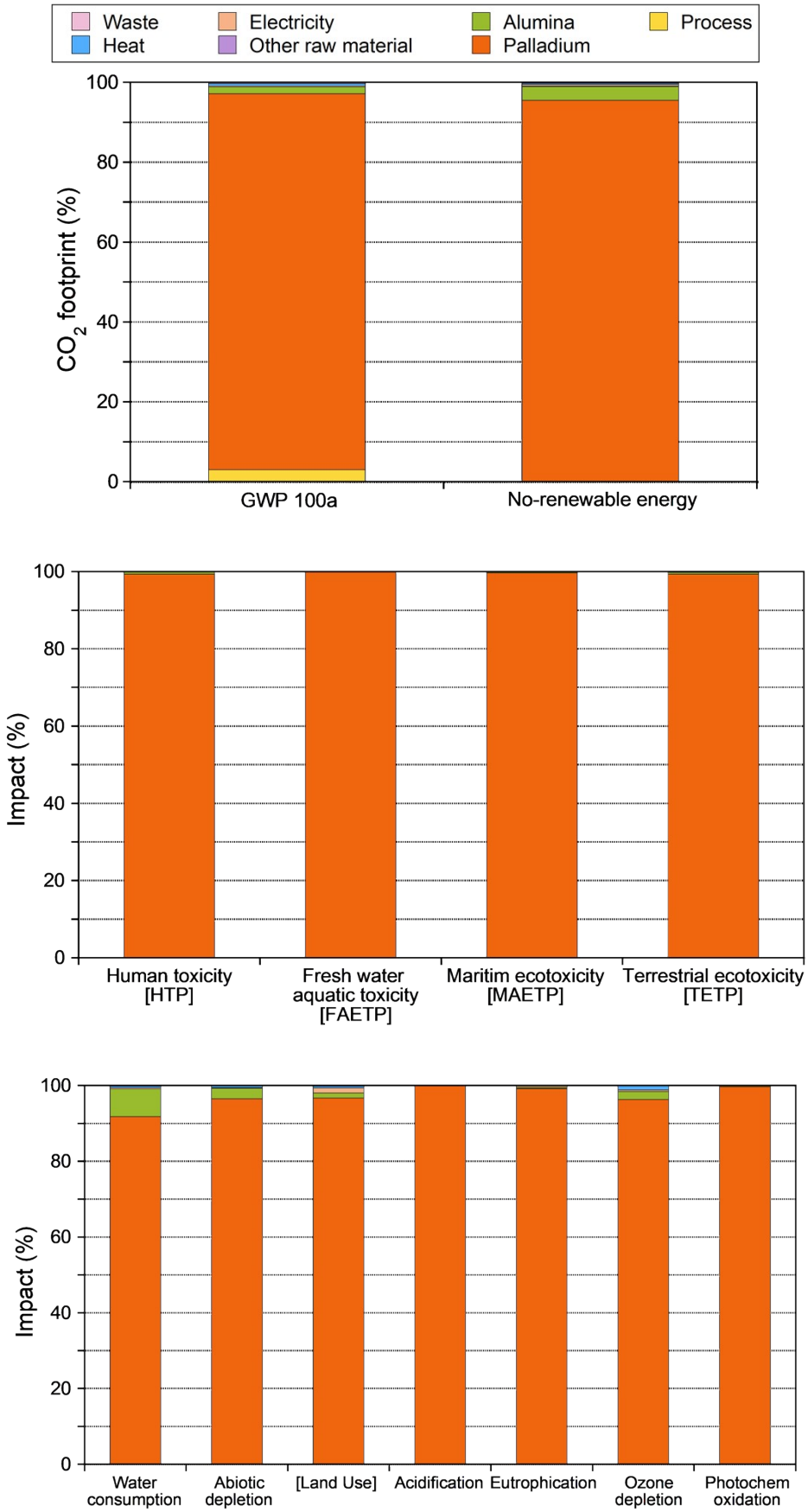
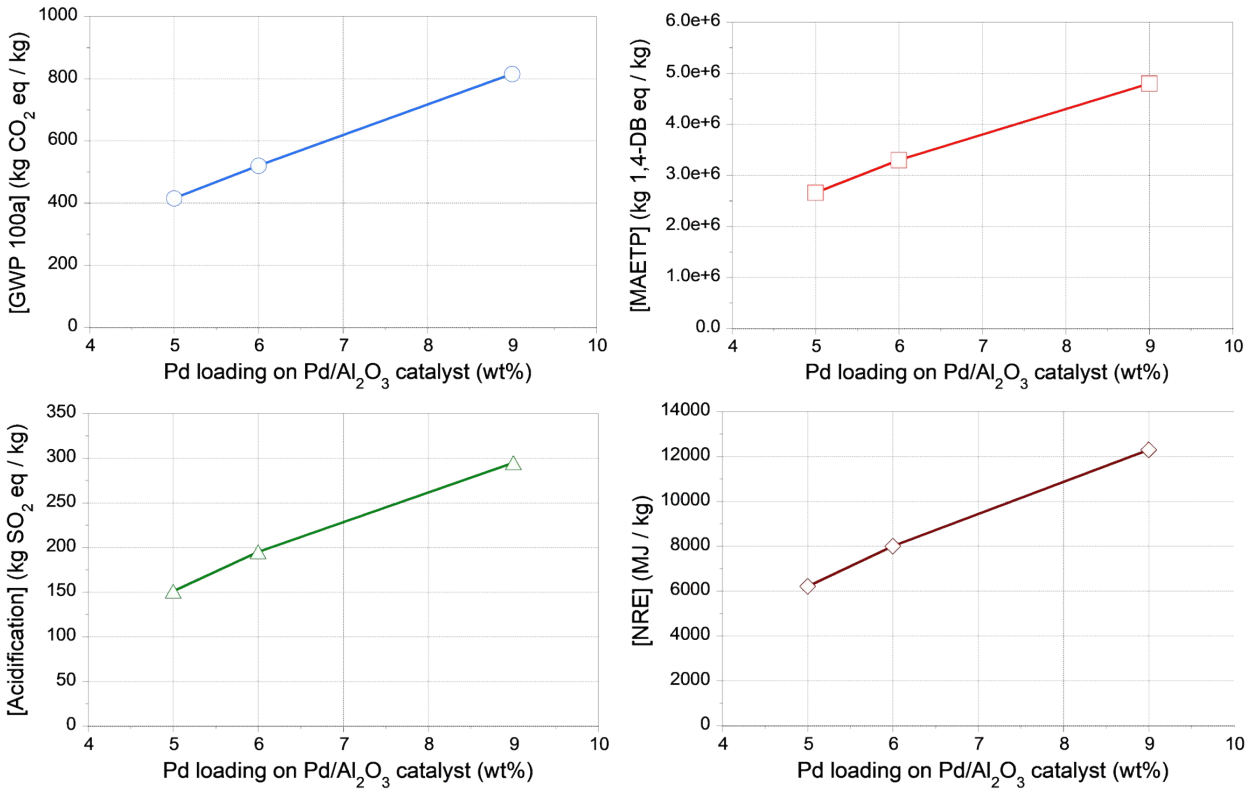


Fig S5. Contributions to environmental impacts for the manufacture of THF-ALD-1.



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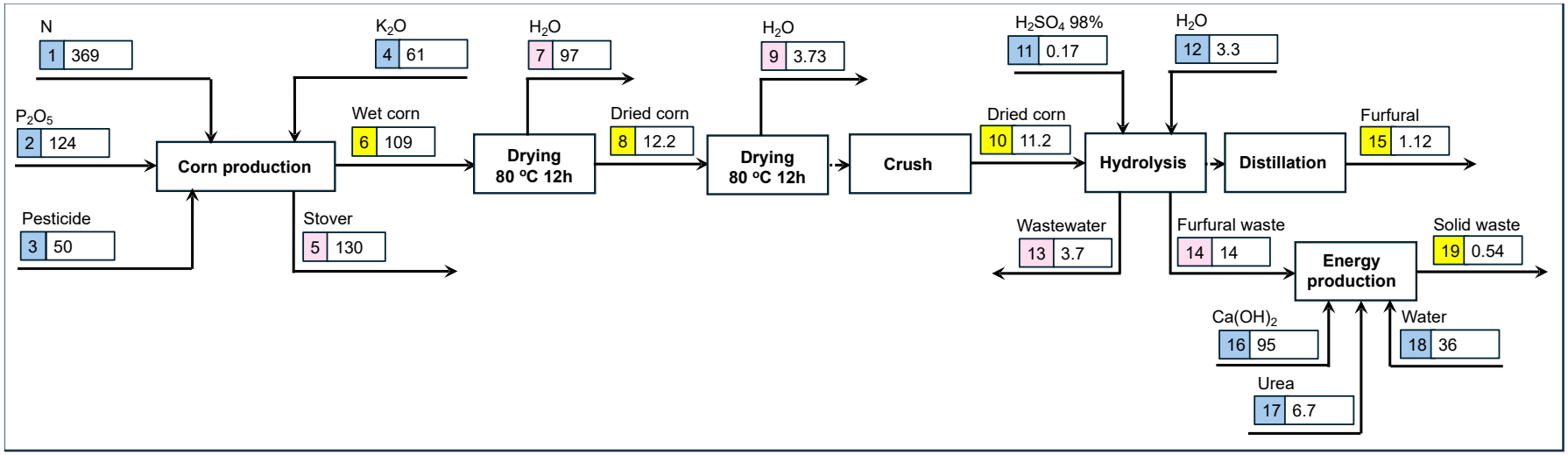
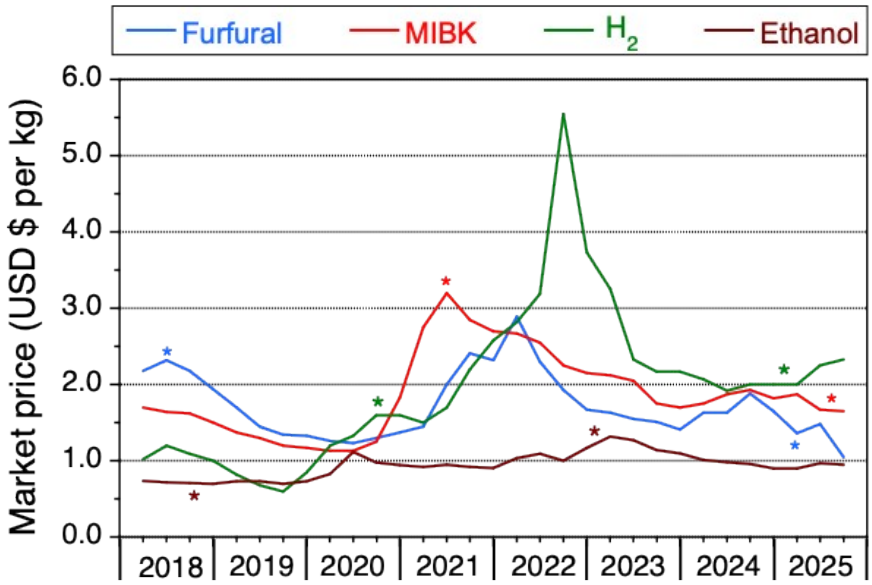


Fig S7. Flowsheet for manufacturing FF from corn. Process adapted from ref[S2].



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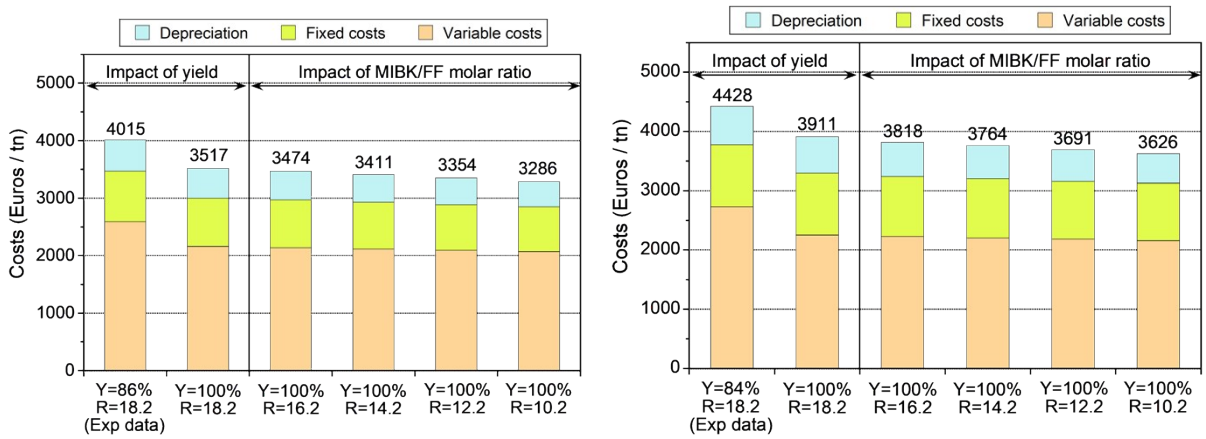

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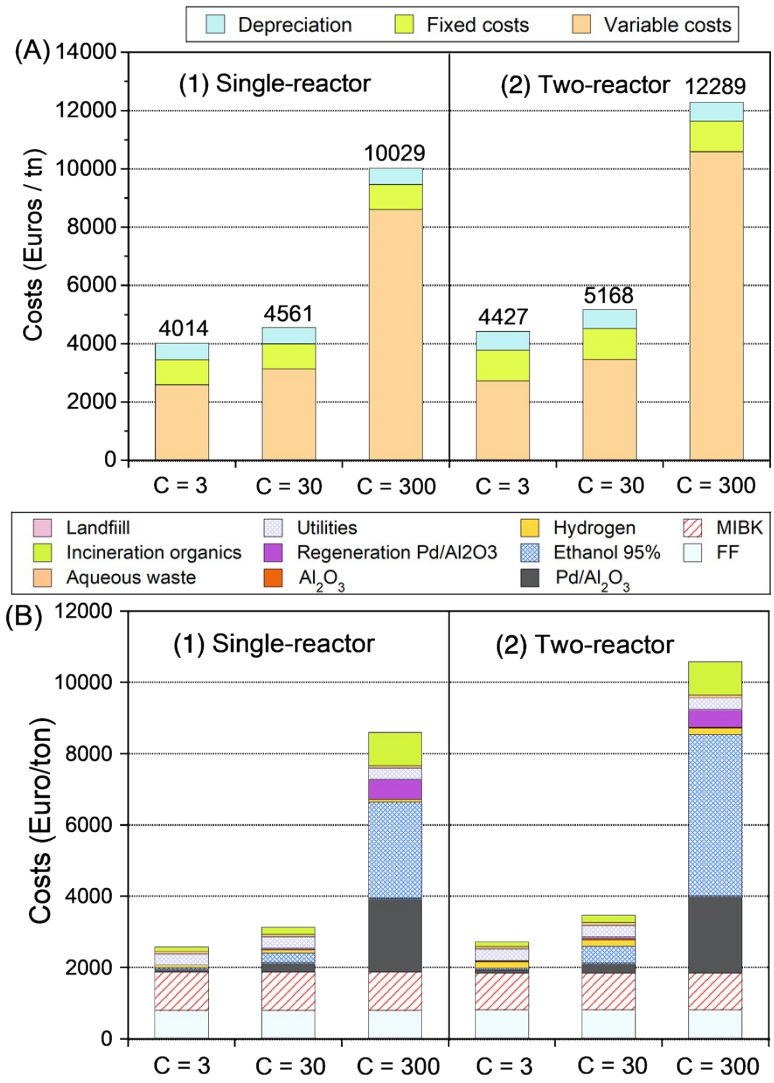

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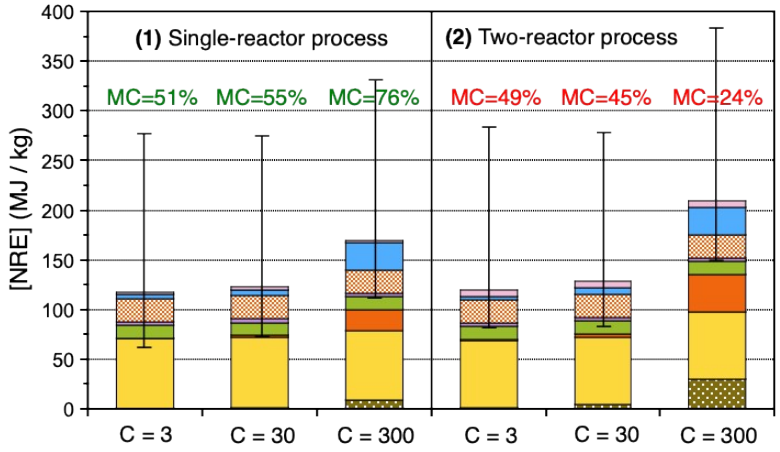

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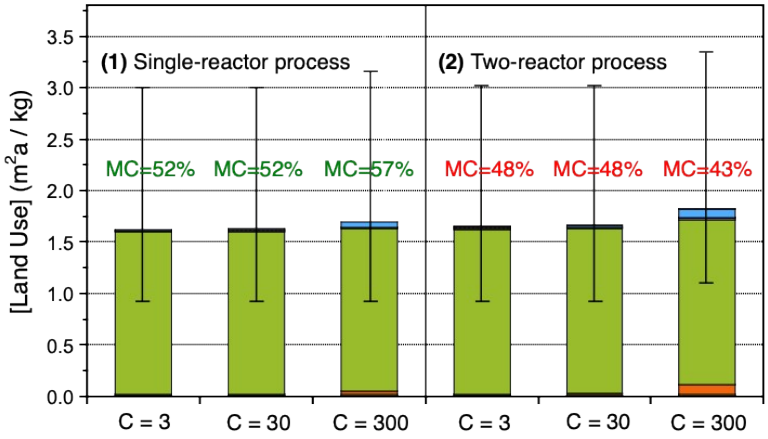

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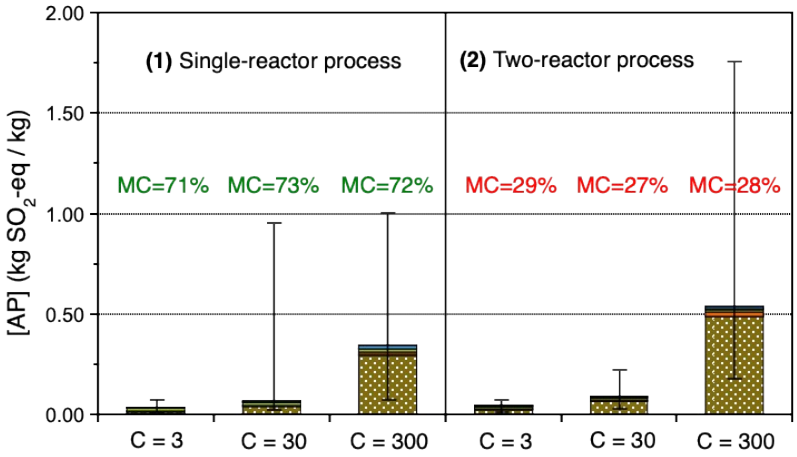

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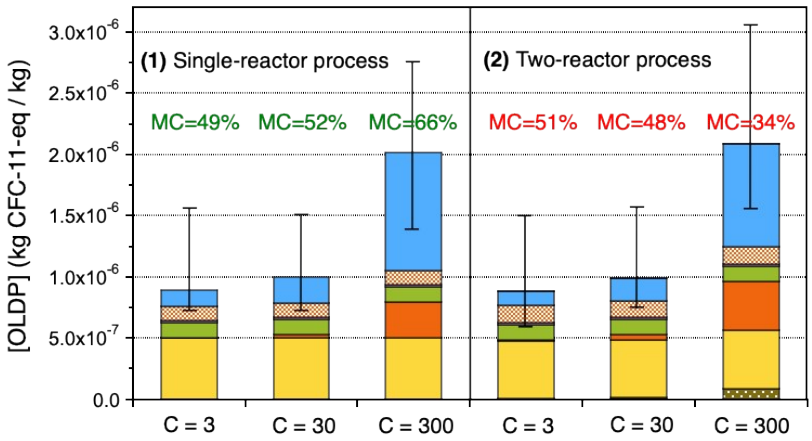

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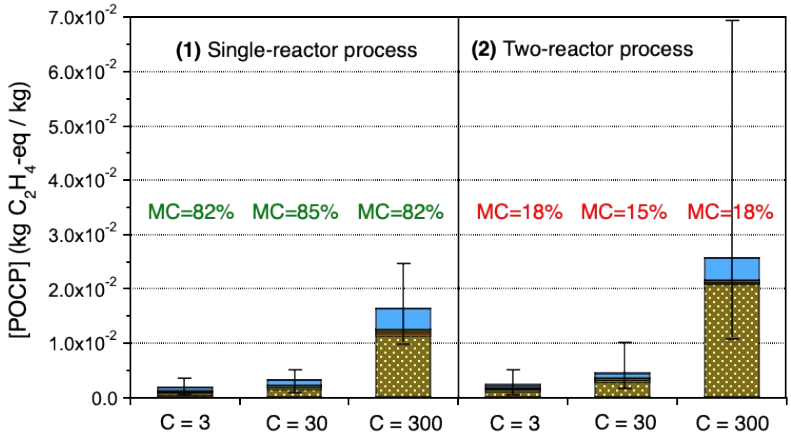

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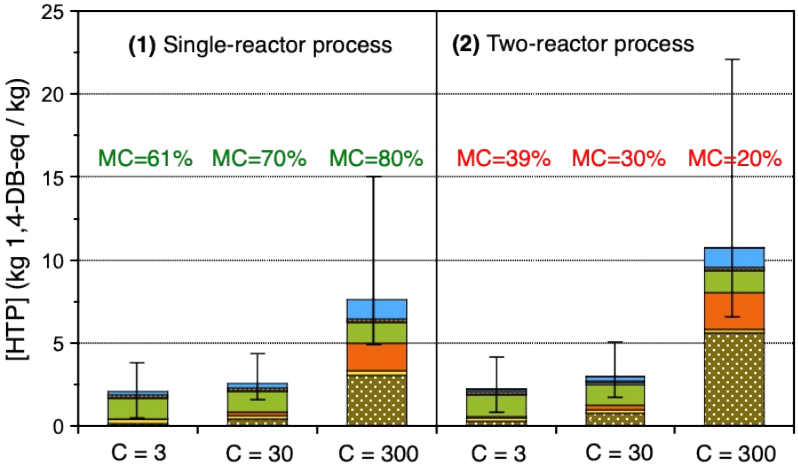

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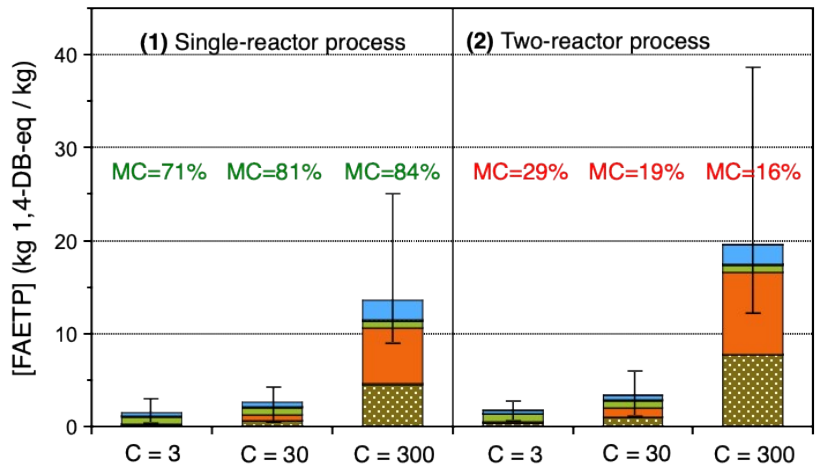

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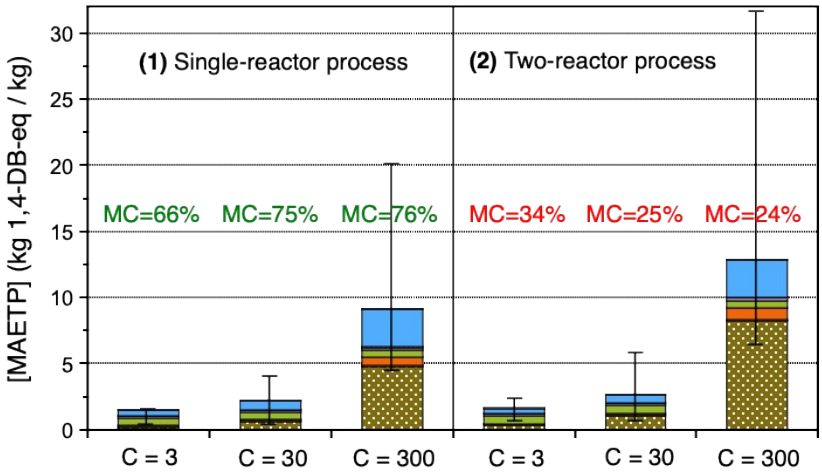

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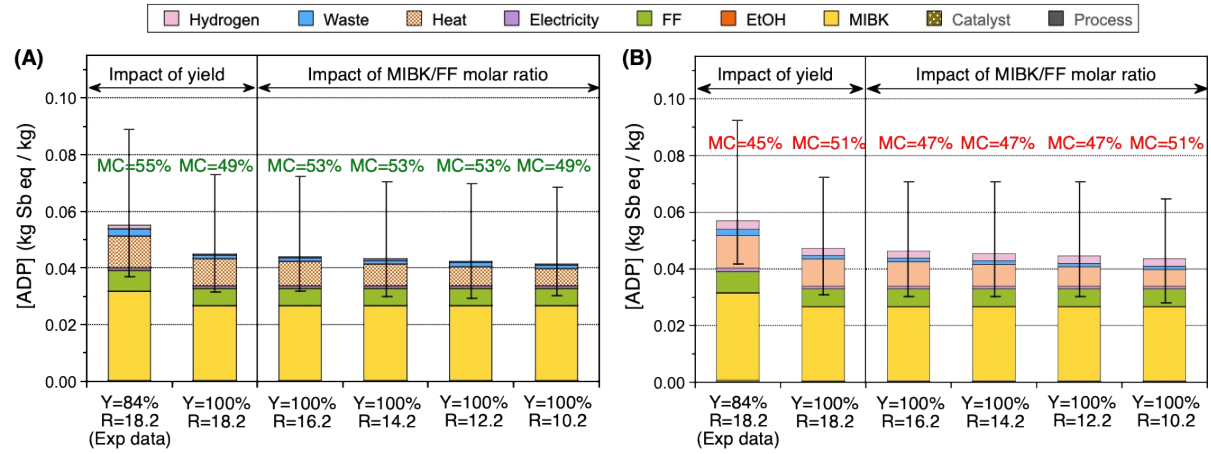

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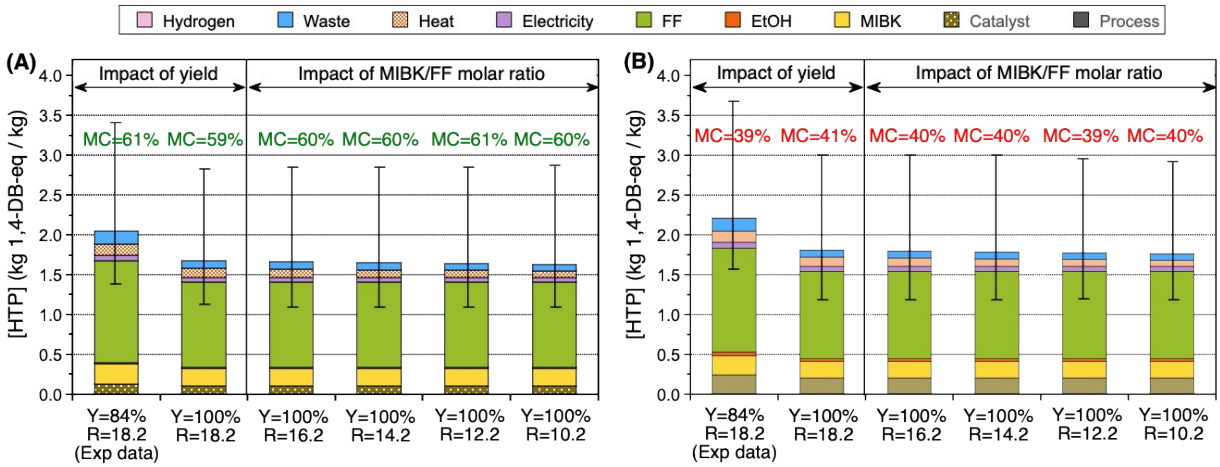

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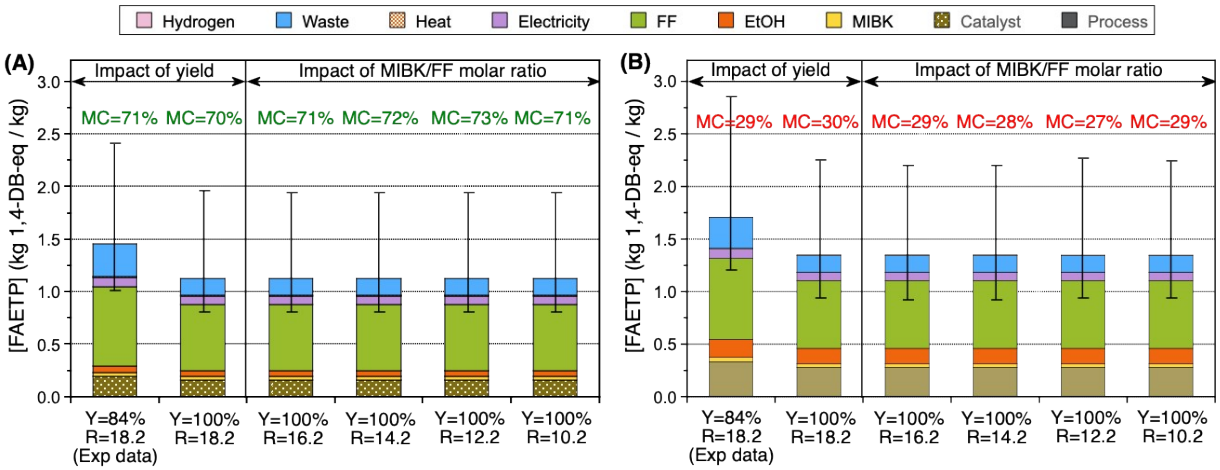

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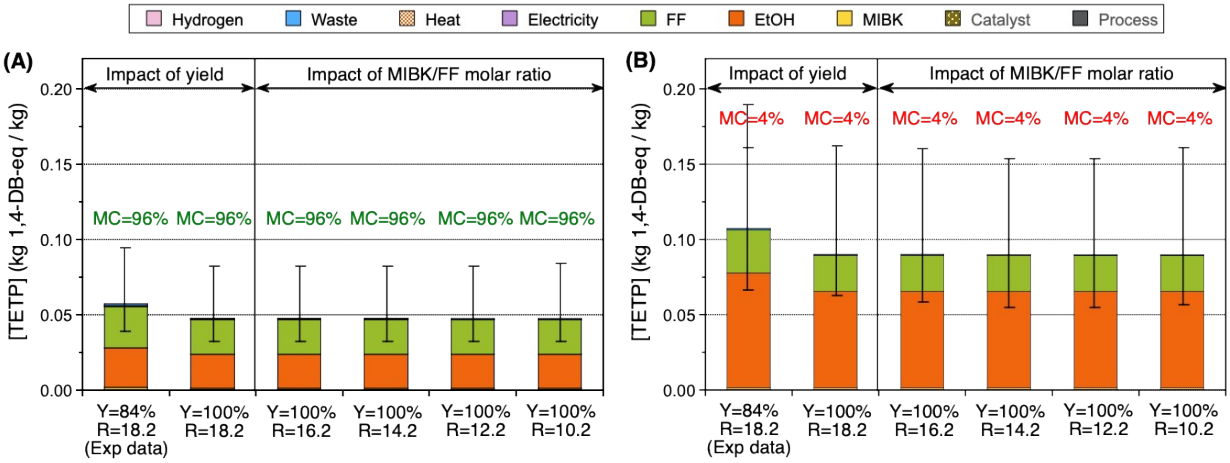

Fig S22. Effect of the overall yield and MIBK/FF molar ratio on Terrestrial Ecotoxicity Potential [TETP] for (1) single-reactor and (2) two-reactor processes (C=3). The error bars were measured as the 2.5th and 97.5th percentiles (95% confidence interval). The number on top of the bars indicate the percentage of MC calculations favouring either the single-reactor or two-reactor scenarios.

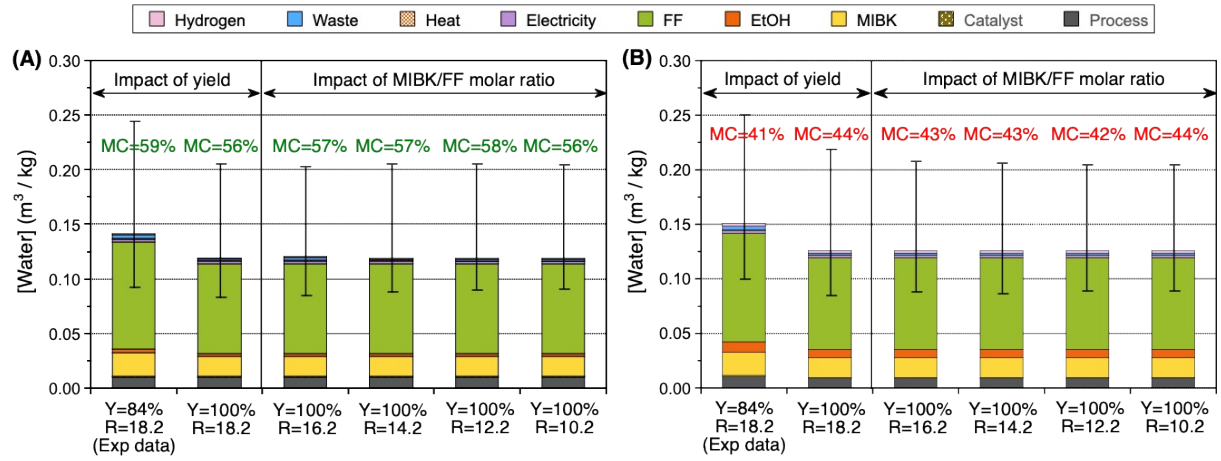

Fig S23. Effect of the overall yield and MIBK/FF molar ratio on Water Consumption [Water] for (1) single-reactor and (2) two-reactor processes (C=3). The error bars were measured as the 2.5th and 97.5th percentiles (95% confidence interval). The number on top of the bars indicate the percentage of MC calculations favouring either the single-reactor or two-reactor scenarios.

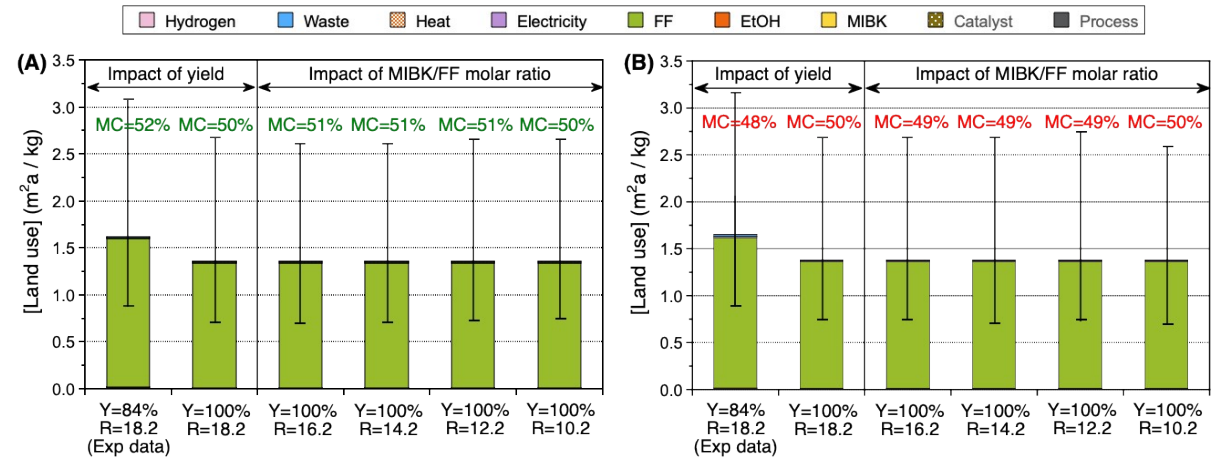

Fig S24. Effect of the overall yield and MIBK/FF molar ratio on Land [Land Use] for (1) single-reactor and (2) two-reactor processes (C=3). The error bars were measured as the 2.5th and 97.5th percentiles (95% confidence interval). The number on top of the bars indicate the percentage of MC calculations favouring either the single-reactor or two-reactor scenarios.

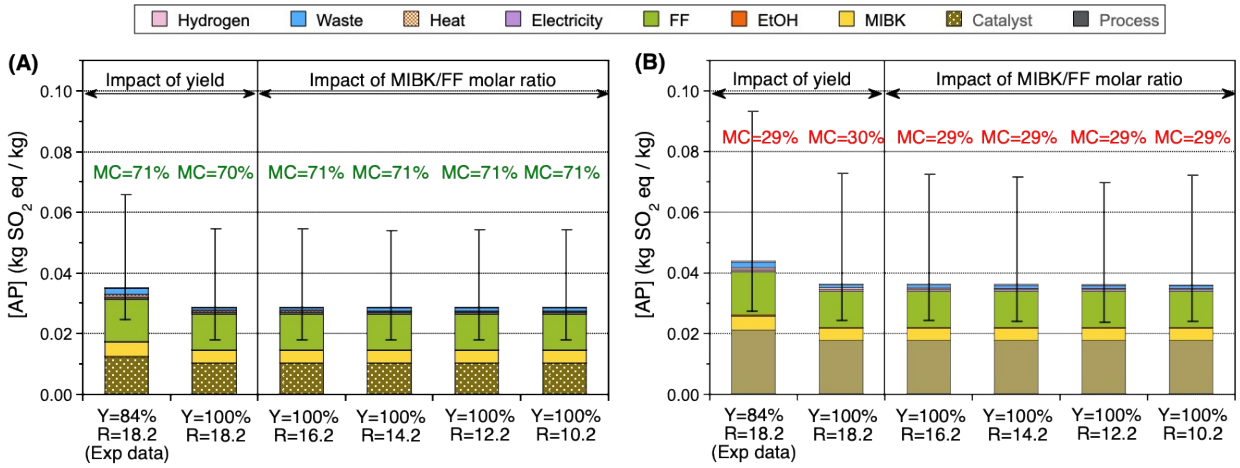

Fig S25. Effect of the overall yield and MIBK/FF molar ratio on Acidification Potential [AP] for (1) single-reactor and (2) two-reactor processes (C=3). The error bars were measured as the 2.5th and 97.5th percentiles (95% confidence interval). The number on top of the bars indicate the percentage of MC calculations favouring either the single-reactor or two-reactor scenarios.

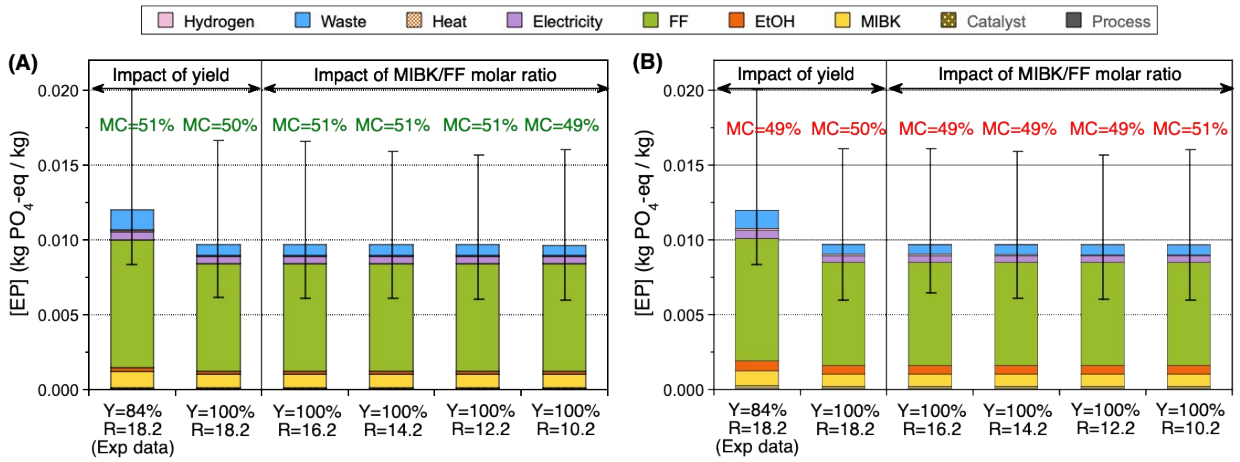

Fig S26. Effect of the overall yield and MIBK/FF molar ratio on Eutrophication Potential [EP] for (1) single-reactor and (2) two-reactor processes (C=3). The error bars were measured as the 2.5th and 97.5th percentiles (95% confidence interval). The number on top of the bars indicate the percentage of MC calculations favouring either the single-reactor or two-reactor scenarios.

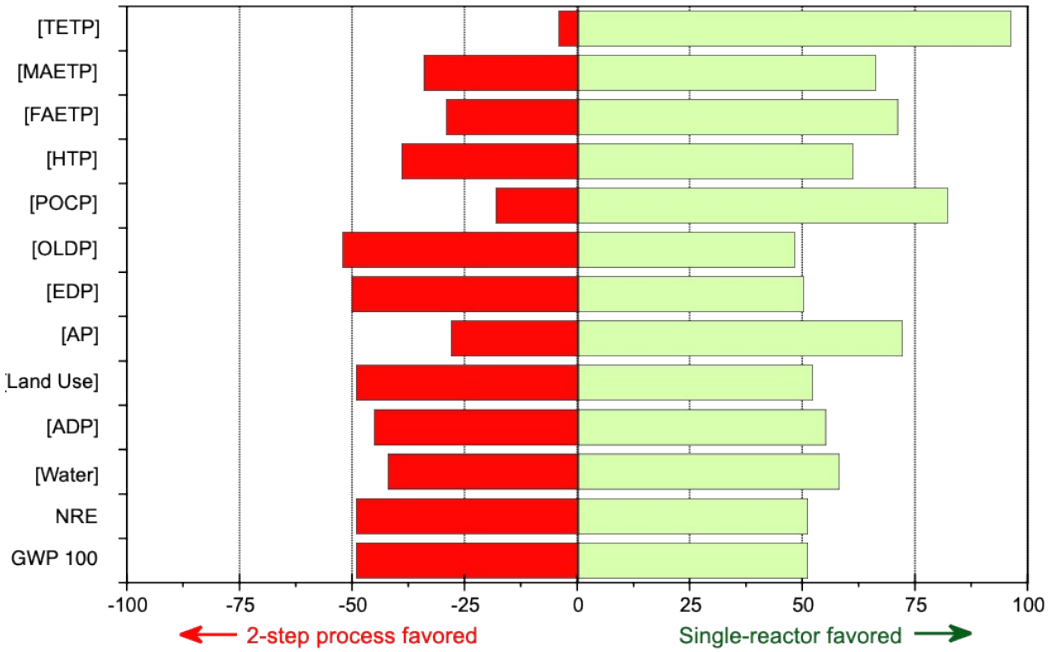

Fig S27. Uncertainty analysis for the single-reactor (green) and two-reactor (red)-processes issued from Monte Carlo analysis unveiling the statistical significance of the average values measures for the different impact categories (base case).

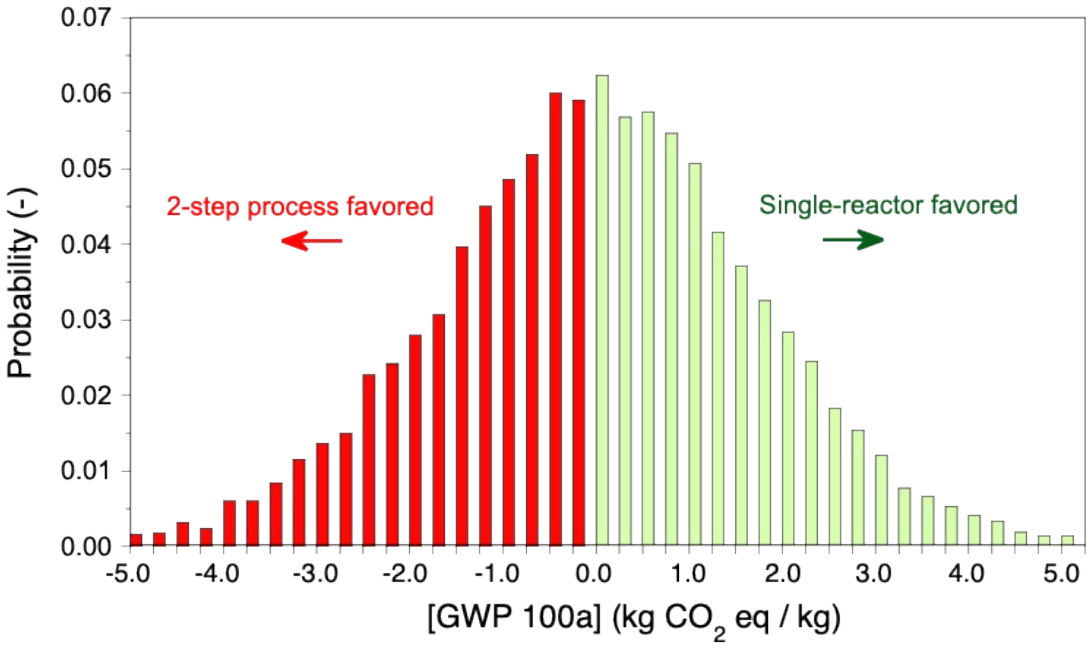

Fig S28. Log-normal plot issued from Monte Carlo analysis for Climate Change [GWP 100a] comparing the single-reactor and two-step processes.

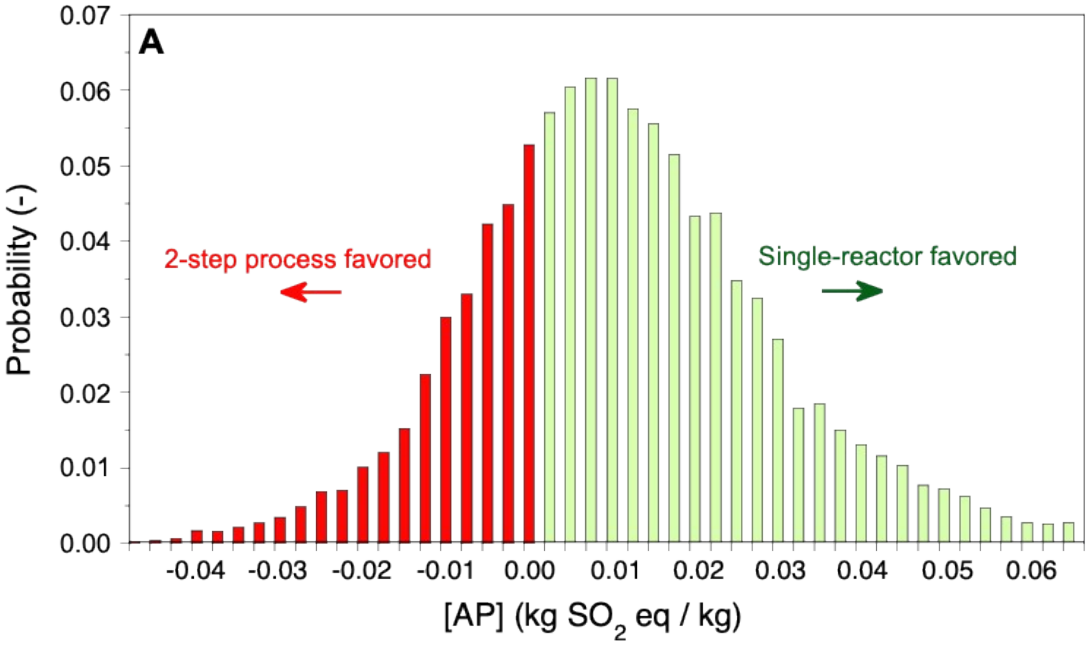

Fig S29. Log-normal plot issued from Monte Carlo analysis for Acidification [AP] comparing the single-reactor and two-step processes.

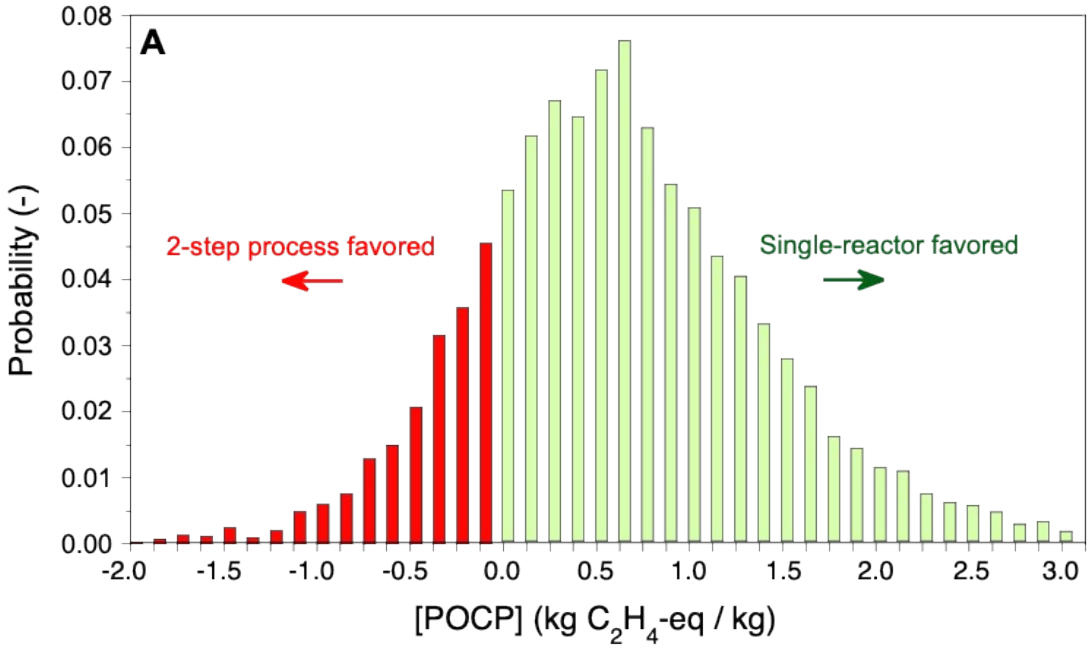

Fig S30. Log-normal plot issued from Monte Carlo analysis for Photochemical Oxidation [POCP] comparing the single-reactor and two-step processes.

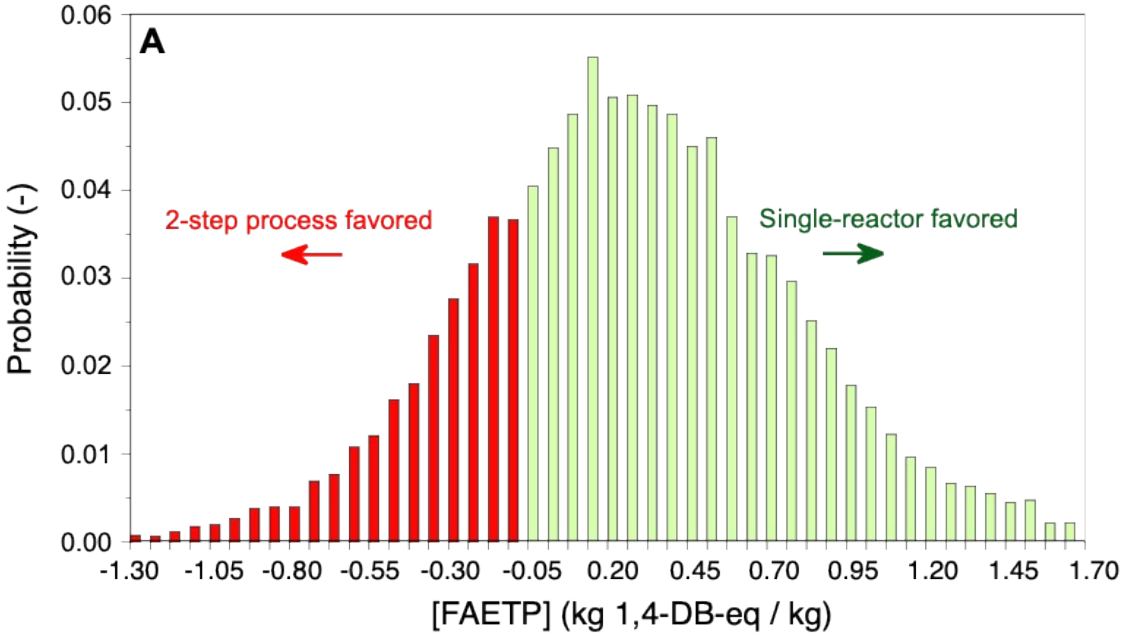

Fig S31. Log-normal plot issued from Monte Carlo analysis for Freshwater Aquatic Ecotoxicity [FAETP] comparing the single-reactor and two-step processes.

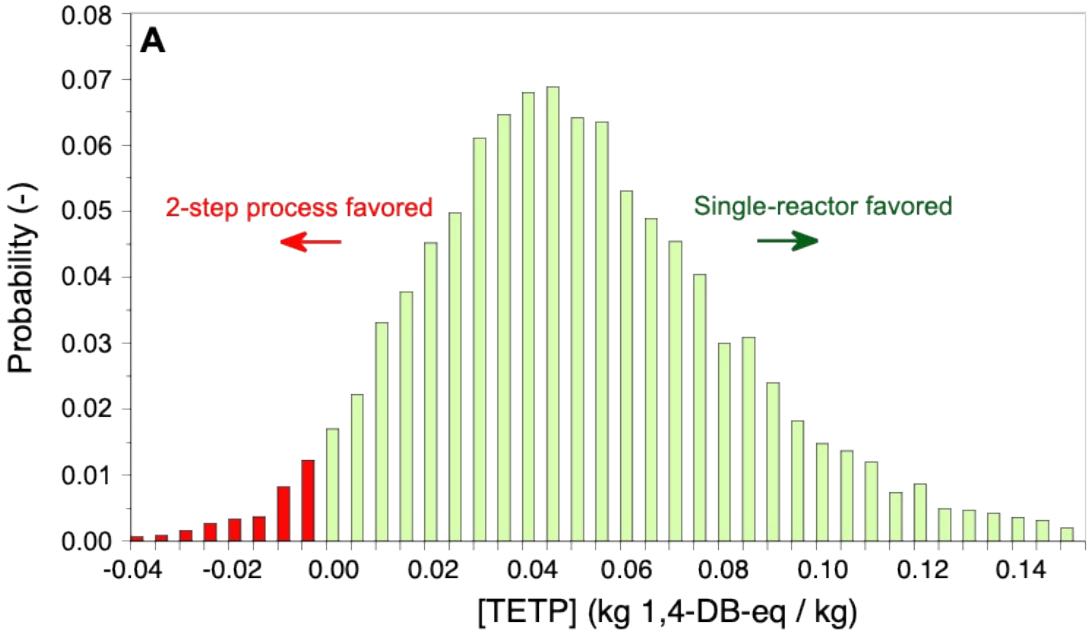

Fig S32. Log-normal plot issued from Monte Carlo analysis for Terrestrial Aquatic Ecotoxicity [TETP] comparing the single-reactor and two-step processes.

Table S1. Physicochemical properties of the main chemicals for THF-ALD-1 manufacture in single-reactor and two-reactor process

Chemical	Specific heat ($J.g^{-1}.°C^{-1}$)*	Enthalpy of vapor. (kJ/kg)**	Boiling T (°C)	Density ($g.cm^{-3}$)	M_W ($g.mol^{-1}$)
FF	1.15	365.0	161.7	1.16	96.09
MIBK	2.15	331.0	116.2	0.802	100.18
ALD-1	1.11	204.5	96.5	-	178.20
ALD-2	0.726	279.3	471.8	-	278.40
THF-ALD-1	1.88	279.5	263.8	-	184.30
THF-ALD-2	1.26	265.0	463.9	-	282.40
Toluene	1.70	360.7	110.6	0.87	92.14
Ethanol	2.44	838.0	78.3	0.79	46.07
Water	4.18	2257	100.0	0.99	18.01

* Values at 20 °C; ** Values at boiling point

Table S2. Process inventory of FFDA production from FF and MIBK in single-reactor and two-step process. Calculations scaled for a production of 3,300 ton/year

Inventory	Items and their unit	Single-reactor process		Two-reactor process	
		UF**	Variable cost (€/ton)	UF**	Variable cost (€/ton)
Raw Materials	FF	0.618	804	0.629	817
	MIBK	0.859	1074	0.822	1028
	H_2	0.039	78	0.091	182
	Ethanol 95%	0.0090x3	27	0.0270x3	45
Catalysts	Al_2O_3	-	-	0.00258	23
	Pd/Al_2O_3	0.00009	87	0.00010	94
Utilities	Steam	10.1	252	10.7	268
	Electricity	0.41	32	0.41	33
	Cooling water	512	26	544	27
	Process water	-	-	-	-
Waste	Total aqueous waste	0.108	76	0.110	77
	Total incineration waste	0.412	130	0.403	121
	Total landfill	0.0000279	0	0.0001652	0.1
Catalyst regeneration	Al_2O_3	-	-	-	-
	Pd/Al_2O_3 (3 cycles / year)	0.000279	5.6	0.000242	5.0
TOTAL COSTS			**2591**		**2726**

* Unit cost expressed in €/ton for raw materials, catalysts, and catalyst regeneration and steam, €/MWh for electricity, and €/m^3 for cooling and process water

** UF (usage factor) = quantity of material / utility per 1 ton of finished good – Electricity in MWh – water in m^3 – all other materials and steam in ton

Table S3. Summary of process assumptions for the manufacture of THF-ALD-1 in single-reactor and two-reactor process

Process	**Single-reactor process**			**Two-step process**		
Aldol condensation						
Ratio MIBK / FF (mol/mol)	18.2			18.2		
Ratio (Pd)Al_2O_3/FF (w:w)	20%			20%		
Time / T / P	3 h	180 °C	5.0 bar	3 h	180 °C	5.0 bar
FF conversion	92%			93%		
ALD-1 / ALD-2 selectivity	100%	0%		92.5%	7.5%	
Hydrogenation						
Excess H_2 (mol)	1.10			1.10		
Ratio Pd/Al_2O_3 / FFAD (w:w)	20%			0%		
Ratio Pd/Al_2O_3 / FF (w:w)	37%			0%		
Time / T / P	3 h	180 °C	20 bar	6 h	180 °C	20 bar
ALD-1 conversion	92%			93%		
THF-ALD-1 / THF-ALD-2 selectivity	100%	0%		100%	100%	
H_2 recycling loop (purge + compression)						
Ratio purge H_2 wt%	100%			100%		
Initial conditions		25 °C	20 bar		25 °C	20 bar
Time / T / P recompression	0.5 h	25 °C	1 bar	0.5 h	25 °C	1 bar
Regeneration catalyst 1						
Loss Al_2O_3 per in mass media	2.0%			-		
Loss Al_2O_3 per regeneration	0.050%			-		
Ratio EtOH / (Pd)Al_2O_3	5			-		
# washings EtOH	1			-		
# of cycles Al_2O_3 before regeneration	3			-		
Initial conditions		25 °C	1 bar		-	-
Time / T / P recompression	1 h	25 °C	1 bar	-	-	-
Regeneration catalyst 2						
Loss Al_2O_3 per in mass media	0.05%			0.05%		
Loss Al_2O_3 per regeneration	0.0050%			0.0050%		
Ratio EtOH / (Pd)Al_2O_3	5			5		
# washings EtOH	1			1		
# of cycles Al_2O_3 before regeneration	3			3		
Initial conditions		25 °C	1 bar		25 °C	1 bar
Time / T / P recompression	1 h	25 °C	1 bar	1 h	25 °C	1 bar
Reactivation catalyst 2						
Loss Pd/Al_2O_3 after reactivation	0.0%			0.0%		
Ratio reactant per Pd/Al_2O_3	13.889			0.0		
No cycles Pd/Al_2O_3 before reactivation	3			1		
Initial conditions		25 °C	1 bar		25 °C	1 bar
Time / T / P recompression	2 h	550 °C	20 bar	1 h	200 °C	1 bar

Table S3. (to be continued)

Process	Single-reactor process			Two-step process		
Azeotropic distillation + MIBK						
Water amount in azeotrope (wt%)	24%			24%		
MIBK solubility in water (wt%)	2.0%			2.0%		
Water solubility in MIBK (wt%)	1.6%			1.6%		
Initial conditions		25 °C	1.0 bar		25 °C	1.0 bar
Time / T / P	3 h	88 °C	1.0 bar	3 h	88 °C	1.0 bar
Recycling loop	0.5 h	20 °C	1.0 bar	0.5 h	20 °C	1.0 bar
Toluene distillation						
Initial conditions		88 °C	1.0 bar		88 °C	1.0 bar
Time / T / P	3 h	111 °C	1.0 bar	3 h	111 °C	1.0 bar
Toluene rate of recovery	98%			98%		
Recycling loop	0.5 h	20 °C	1.0 bar	0.5 h	20 °C	1.0 bar
MIBK distillation						
Initial conditions		111 °C	1.0 bar		111 °C	1.0 bar
Time / T / P	3 h	116 °C	1.0 bar	3 h	116 °C	1.0 bar
Toluene rate of recovery	98%			98%		
Recycling loop	0.5 h	20 °C	1.0 bar	0.5 h	20 °C	1.0 bar
FF distillation + lights						
Initial conditions		116 °C	1.0 bar		116 °C	1.0 bar
Time / T / P	3 h	162 °C	1.0 bar	3 h	162 °C	1.0 bar
Toluene rate of recovery	0%			0%		
Recycling loop	0.5 h	20 °C	1.0 bar	0.5 h	20 °C	1.0 bar
Heavy products distillation						
Initial conditions		100 °C	1.0 bar		116 °C	1.0 bar
Time / T / P	3 h	110 °C	0.012 bar	3 h	110 °C	0.012 bar
Toluene rate of recovery	98%			98%		
Recycling loop	0.5 h	20 °C	1.0 bar	0.5 h	20 °C	1.0 bar
THF-ALD-1 distillation						
Initial conditions		160 °C	1.0 bar		160 °C	1.0 bar
Time / T / P	3 h	180 °C	0.090 bar	3 h	180 °C	0.090 bar
Toluene rate of recovery	98%			98%		
Yield 2nd step after distillation	90.2%			98.0%		
Global yield	82.9%			84.3%		
EtOH 95% distillation						
Initial conditions		25 °C	1.0 bar		25 °C	1.0 bar
Time / T / P	3 h	78 °C	1.0 bar	3 h	78 °C	1.0 bar
Toluene rate of recovery	98%			98%		
Yield 2nd step after distillation	95%			95%		

Table S4. Key background datasets using in the LCI and corresponding Ecoinvent version

Background process / Material	Dataset Name (Ecoinvent)	Version	Region / Market	Notes
Maize	Market for Maize*	v3.4	GLO	Global market
MIBK	Market for MIBK	v3.6	GLO	Global market
Ethanol	Market for ethanol	v3.6	GLO	Global market
Palladium	Market for Maize	v3.4	GLO	Global market
Alumina (HP Ziegler process)	Alumina, HP Ziegler	v3.6	RER	European proxy dataset
Electricity	Medium voltage electricity	v3.4	RER	Harmonized European mix
Steam / Heat	Heat, industrial, natural gas, >100 kW	v3.6	Europe without Switzerland	Repesentative European boiler
Process/cooling water	Water, at user	v3.6	RER	European average
Hydrogen	Hydrogen, gaseous	v3.6	GLO	Global market

* From Agri-footprint database adapted to Ecoinvent 3.4

Table S5. Revised Pd inventories (in blue). From these values, all impacts in Ecoinvent 3.4 were multiplied by 1.7 compared to the existing inventories*

No	Impact category	Unit	Pd {GLO} market (2002)	Pd {GLO} market (2019)	Pd {ZA} PGM mine (2019)	Pd {RU} PGM mine (2019)	Pd {RER} automobile catalyst (2019)	Pd {ROW} automobile catalyst (2019)
1	GWP 100a	kg CO_2-eq	**4900**	**8252**	16773	7235	382	640
	Trapped biogenic CO_2 [Biogenic CO_2]	kg CO_2-eq	0	0	0	0	0	0
2.1	Non-renewable energy	MJ primary	**65000**	**109669**	198798	116359	6890	7426
	- Nuclear energy [Uranium]	MJ	6290	10588	11299	17325	2854	798
	- Coal energy [Coal]	MJ	35100	59106	157435	21627	2353	3996
	- Crude oil energy [Oil]	MJ	5570	9382	18845	8459	365	666
	- Natural gas energy [Gas]	MJ	18400	31100	12556	69125	1336	2031
2.2	Renewable energy resources [Renew]	MJ	2060	3469	3698	5455	965	613
	- Primary forest energy [Primary Forest]	MJ	0	0	0	1	0	0
3.1	Human toxicity [HTP]	kg 1,4-DB-eq	13300	22420	55606	12398	288	357
3.2	Freshwater aquatic ecotoxicity [FAETP]	kg 1,4-DB-eq	16280	27420	49721	30342	198	217
3.3	Marine ecotoxicity [MAETP]	kg 1,4-DB-eq	**28704230**	**48340267**	11987016	31778477	444592	500598
3.4	Terrestrial ecotoxicity [TETP]	kg 1,4-DB-eq	17.80	30	53	35	1	2
4	Water consumption	m^3	47	79	76	141	5	3
5	Abiotic depletion	kg Sb-eq	37	62	126	54	2	4
6	Quantitative land use [Land Use]	m^2a	67	113	208	114	31	4
7	Acidification	kg SO_2-eq	1820	3064	295	7729	2	3
8	Eutrophication	kg PO_4-eq	36	61	168	19	1	1
9	Ozone depletion	kg CFC-11-eq	0	0	0	0	0	0
10	Photochemical oxidation	kg C_2H_4-eq	72	122	11	309	0	0

* Nomenclature: GLO = global; ZA = South Africa; RU = Russia; RER = Rest of Europe; ROW = Rest of the World; PGM = Platinum Group Metal

Table S6. Process inventory to produce 5wt%Pd/Al_2O_3.

Inventory	Items and their unit	UF*
Raw Materials	A_1 Palladium	0.0500
	A_2 HNO_3 in water (60%)	0.2017
	A_3 AlOOH	1.3007
	A_4 H_2	0.0132
	A_5 H_2O	2.3308
	A_6 NH_3	0.0167
Utilities	A_7 Steam	5
	A_8 Electricity	0.55
	A_9 Cooling water	8.4
	A_{10} Process water, m^3/h	2.804
Waste	A_{11} Aqueous waste	0.1541
	A_{12} H_2	0.0122
	A_{13} NO_2	0.0432
	A_{14} N_2O	0.0410
	A_{15} Process water	0.0410

* UF (usage factor) = quantity of material / utility per 1 kg of 5wt%Pd/Al_2O_3 – Electricity in kWh – cooling and process water in kg – all other materials and steam in kg

Table S7. Environmental impacts for the manufacture of 5wt%Pd/Al_2O_3 (computed using Ecoinvent database 3.4)

No	Impact category	Unit	5wt%Pd/Al_2O_3 (2019)
1	GWP 100a	kg CO_2-eq	418
	Trapped biogenic CO_2 [Biogenic CO_2]	kg CO_2-eq	0
2.1	Non-renewable energy	MJ primary	6144
	- Nuclear energy [Uranium]	MJ	582
	- Coal energy [Coal]	MJ	3396
	- Crude oil energy [Oil]	MJ	582
	- Natural gas energy [Gas]	MJ	1591
2.2.	Renewable energy resources [Renew]	MJ	183
	- Primary forest energy [Primary Forest]	MJ	0.0203
3.1	Human toxicity [HTP]	kg 1,4-DB eq	1642
3.2	Freshwater aquatic ecotoxicity [FAETP]	kg 1,4-DB eq	2394
3.3	Marine ecotoxicity [MAETP]	kg 1,4-DB eq	2525680
3.4	Terrestrial ecotoxicity [TETP]	kg 1,4-DB eq	2.3
4	Water consumption	m^3	4.2
5	Abiotic depletion	kg Sb-eq	3.5
6	Quantitative land use [Land Use]	m^2a	7.4
7	Acidification	kg SO_2-eq	154
8	Eutrophication	kg PO_4-eq	1.9
9	Ozone depletion	kg CFC-11-eq	0.000022
10	Photochemical oxidation	kg C_2H_4-eq	6.1

Table S8. Amount of Pd reused and cost as a function of the number of regeneration cycles (C) of Pd/Al_2O_3 catalyst

C	Single-reactor		Two-reactor	
	Pd/THF-ALD-1 (g/ton)	Pd/Al_2O_3 cost (€/ton)	Pd/THF-ALD-1 (g/ton)	Pd/Al_2O_3 cost (€/ton)
3	5.9	88	6.5	97
30	18.3	273	20.4	303
300	142.9	2127	158.8	2363

* Production = 3300 ton/year of THF-ALD-1

Table S9. Process inventory for the manufacture of FF

Inventory	Items and their unit	UF*
Raw Materials	A_1 Fertilizer (N)	369
	A_2 P_2O_5	124
	A_3 Pesticide	50
	A_4 K_2O	61
	A_5 H_2SO_4 (98%)	0.17
	A_6 H_2O	3.4
	A_7 Lime	95
	A_8 Urea	6.7
	A_9 H_2O	39
Utilities	A_{10} Steam	40
	A_{11} Electricity	21
Waste	A_{12} Stove	130
	A_{13} Wastewater	10
	A_{14} Inert waste	14

* UF (usage factor) = quantity of material / utility per 1.12 of FF – Electricity in MWh – wastewater in m^3 – all other materials and steam in ton

Table S10. Pedigree matrix with the scores used to assess the quality of data sources (readapted from ref.[S7])

Score	1	2	3	4	5
U1 Reliability	Verified data based on measurements	Verified data partly based on assumptions or non-verified data based on measurements	Non-verified data partly based on qualified estimates	Qualified estimate (*e.g.*, by industrial expert)	Non-qualified estimate
	1.00	**1.05**	**1.10**	**1.20**	**1.50**
U2 Completeness	Representative data from all sites relevant for market considered over adequate period to even out normal fluctuations	Representative data from >50% of sites relevant for market considered over adequate period to even out normal fluctuations	Representative data from only some relevant sites (<<50%) or >50% of sites but from shorter periods	Representative data from only one relevant site or some sites but from shorter periods	Representativeness unknown or data from a small number of sites and shorter periods
	1.00	**1.02**	**1.05**	**1.10**	**1.20**
U3 Temporal correlation	< 3 years difference to time period of the dataset	<6 years difference to time period of the dataset	<10 years difference to time period of the dataset	<15 years difference to time period of the dataset	Age of data unknown or >15 years difference to time period of the dataset
	1.00	**1.03**	**1.10**	**1.20**	**1.50**
U4 Geographical correlation	Data from area under study	Average data from larger area in which the area under study is included	Data from area with similar production conditions	Data from area with slightly similar production conditions	Data from unknown or distinctly different area
	1.00	**1.01**	**1.02**	**1.05**	**1.10**
U5 Further technological correlation	Data from enterprises, processes and materials under study	Data from processes/materials under study but from different enterprises	Data from processes/materials under study but different technology	Data on related processes or materials	Data on related processes on laboratory scale or from different technology
	1.00	**1.05**	**1.20**	**1.50**	**2.00**

Table S11. Scores used for the Pedigree matrix to assess the quality of data sources for two-step and single-reactor processes (derived from ref.[S7])

Input parameter	U1	U2	U3	U4	U5	U6	SD	GSD
Process	1	2	3	2	2	0.3000	0.5897	1.803
Catalysts	1	2	3	2	2	0.0006	0.5897	1.803
MIBK	1	2	2	2	1	0.0006	0.3444	1.411
EtOH	1	2	2	2	1	0.0006	0.3444	1.411
FF	1	2	2	2	1	0.0006	0.3444	1.411
Electricity	1	2	2	2	1	0.0006	0.3444	1.411
Heat	1	2	2	2	1	0.0006	0.3444	1.411
Waste	1	2	2	2	1	0.0400	0.3444	1.411
Hydrogen	1	2	2	2	1	0.0060	0.3444	1.411

Table S12. Breakdown of fixed and variable (base case) costs, ~~and~~ depreciation and discounted flow analysis for single-reactor and two-reactor processes.

Process	**(A) SINGLE-REACTOR**			**(B) TWO-REACTOR**		
Fixed cost			**M€**			**M€**
Labour	Shift position	2.4	0.97	Shift position	3.0	1.21
Maintenance	ISBL (%)	5.0	0.55	ISBL (%)	5.0	0.64
Miscellaneous + overheads	% of labour + maintenance	70	1.07	% of labour + maintenance	70	1.30
TOTAL FIXED COSTS	**Step**		**2.59**			**3.14**
CAPEX			**M€**			**M€**
Main equipment (ISBL)			10.9			12.8
OSBL equipment			5.0			5.5
Pd/Al_2O_3 catalyst (4 initial loads)			0.83			0.72
TOTAL CAPEX			**16.7**			**19.0**
Depreciation			**M€**			**M€**
TOTAL DEPRECIATION			**16.7**			**19.0**
	Years	10			10	
TOTAL DEPRECIATION per year	**Step**		**1.67**			**1.90**
FMC (OPEX)			**€/ton**			**€/ton**
Fixed cost + Variable cost + Depreciation			**4015**			**4428**
Discounted cash flow analysis			**€/ton**			**€/ton**
Minimum selling price (MSP)*			**4923**			**5286**

* Internal rate of return (IRR) = 15%

Table S13. Sensitivity analysis for the FMC of THF-ALD-1 as a function of the number of regeneration cycles of the Pd/Al_2O_3 catalyst, overall yield (Y) and MIBK/FF molar ratio (R) in the single-reactor process. Costs given in €/ton

Condition	Variable costs	Gain VC%	Fixed costs	Depreciation	Gain Capex	FMC	Gain FMC %	SPM	Gain SPM%
Y=86%, R=18.2, C=3 (Base case)	2591	0	880	544	0	4015	0	2738	0
Y=86%, R=18.2, C=30	3138	+21%	880	544	0	4562	+14%	2991	+9%
Y=86%, R=18.2, C=300	8606	+174%	880	544	0	10030	+120%	5941	+99%
Y=100%, R=18.2, C=3	2160	-17%	838	519	-7%	3517	-12%	2286	-17%
Y=100%, R=16.2, C=3	2138	-1%	831	504	-4%	3473	-1%	2244	-2%
Y=100%, R=14.2, C=3	2115	-1%	815	481	-4%	3411	-2%	2199	-2%
Y=100%, R=12.2, C=3	2094	-1%	791	469	-4%	3354	-2%	2156	-2%
Y=100%, R=10.2, C=3	2070	-1%	781	435	-7%	3286	-2%	2111	-2%

Table S14. Sensitivity analysis for the FMC of THF-ALD-1 as a function of the number of regeneration cycles of the Pd/Al_2O_3 catalyst, the overall yield (Y) and MIBK/FF molar ratio (R) in the two-reactor process. Costs given in €/ton

Condition	Variable costs	Gain VC%	Fixed costs	Depreciation	Gain Capex	FMC	Gain FMC %	SPM	Gain SPM%
Y=84%, R=18.2, C=3 (Base case)	2727	0	1050	650	0	4427	0	2852	0
Y=84%, R=18.2, C=30	3469	+27	1050	650	0	5169	+17%	3263	+14%
Y=84%, R=18.2, C=300	10590	+205%	1050	650	0	12290	+138%	7565	+131%
Y=100%, R=18.2, C=3	2251	-17%	1050	610	-6%	3911	-12%	2360	-17%
Y=100%, R=16.2, C=3	2228	-1%	1010	580	-5%	3818	-2%	2317	-2%
Y=100%, R=14.2, C=3	2204	-1%	1000	560	-3%	3764	-2%	2269	-2%
Y=100%, R=12.2, C=3	2181	-1%	980	530	-5%	3691	-2%	2226	-2%
Y=100%, R=10.2, C=3	2156	-1%	970	500	-6%	3626	-2%	2178	-2%

Table S15. Sensitivity analysis on the benefits of single-reactor towards two-reactor process for the FMC of THF-ALD-1 as a function of the number of regeneration cycles of the Pd/Al_2O_3 catalyst, the overall yield (Y) and MIBK/FF molar ratio (R). Costs given in €/ton

Condition	Variable costs	Gain VC%	Fixed costs	Depreciation	Gain Capex	FMC	Gain FMC %	SPM	Gain SPM%
Y=86% or 84%, R=18.2, C=3 (Base case)	-136	0%	-190	-90	14%	-416	0%	-114	0%
Y=86% or 84%, R=18.2, C=30	-411	+144%	-190	-90	0	-691	+66%	-272	+140%
Y=86% or 84%, R=18.2, C=300	-1984	+499%	-190	-90	0	-2264	+228%	-1624	+497%
Y=100%, R=18.2, C=3	-91	-33%	-210	-90	15%	-391	-6%	-74	-35%
Y=100%, R=16.2, C=3	-90	-1%	-180	-80	14%	-350	-10%	-72	-3%
Y=100%, R=14.2, C=3	-89	-1%	-180	-80	14%	-349	-1%	-70	-3%
Y=100%, R=12.2, C=3	-88	-1%	-180	-70	13%	-338	-3%	-68	-3%
Y=100%, R=10.2, C=3	-86	-1%	-180	-70	14%	-336	-1%	-66	-3%

Table S16. Breakdown for Non-Renewable Energy [NRE] (in MJ) for single-reactor and two-reactor processes

Energy source	Single-reactor	Two-reactor
Nuclear energy [Uranium]	3.278	3.423
Coal energy [Coal]	10.80	11.15
Crude oil energy [Oil]	56.83	57.01
Natural gas energy [Gas]	46.79	48.46
TOTAL	118	120

Table S17. Sensitivity analysis for the different impact categories for THF-ALD-1 manufacture as a function of the number of recycling cycles of the Pd/Al_2O_3 catalyst (C), overall yield (Y) and MIBK/FF molar ratio (R) in the single-reactor process.

Condition	[GWP 100a] (kg CO_2-eq/kg)	Energy (MJ/kg)		Toxicity (kg 1,4-DB-eq/kg)				[Water] (m^3)	[ADP] (kg Sb-eq/kg)	[Land Use] (m^2a/kg)	[AP] (kg SO_2-eq/kg)	[EP] (kg PO_4-eq/kg)	[OLDP] (kg CFC-11-eq/kg)	[POCP] (kg C_2H_4-eq/kg)
		[NRE]	[Renew]	[HTP]	[FAETP]	[MAETP]	[TETP]							
Y=86%, R=18.2, C=3	6.482	118	-	2.050	1.451	1.472	0.0571	0.141	0.0550	1.621	0.0350	0.0120	$8.940x10^{-7}$	$1.804x10^{-3}$
Y=86%, R=18.2, C=30	7.341	123	-	2.567	2.571	2.189	0.295	0.172	0.0577	1.628	0.0620	0.0151	$1.001x10^{-6}$	$3.170x10^{-3}$
Y=86%, R=18.2, C=300	15.51	170	-	7.629	13.60	9.145	2.676	0.481	0.0830	1.697	0.341	0.0458	$2.018x10^{-6}$	$1.647x10^{-2}$
Y=100%, R=18.2, C=3	5.213	99	-	1.674	1.128	1.116	0.0478	0.118	0.0455	1.360	0.0288	0.0097	$7.110x10^{-7}$	$5.655x10^{-4}$
Y=100%, R=16.2, C=3	5.115	97	-	1.664	1.127	1.115	0.0477	0.118	0.0447	1.360	0.0288	0.0097	$7.022x10^{-7}$	$5.653x10^{-4}$
Y=100%, R=14.2, C=3	5.006	95	-	1.652	1.127	1.113	0.0477	0.118	0.0437	1.360	0.0287	0.0097	$6.924x10^{-7}$	$5.653x10^{-4}$
Y=100%, R=12.2, C=3	4.908	93	-	1.642	1.126	1.112	0.0477	0.118	0.0429	1.359	0.0286	0.0097	$6.836x10^{-7}$	$5.654x10^{-4}$
Y=100%, R=10.2, C=3	4.799	91	-	1.630	1.125	1.110	0.0477	0.118	0.0420	1.359	0.0286	0.0097	$6.739x10^{-7}$	$5.647x10^{-4}$

Table S18. Sensitivity analysis for the different impact categories for THF-ALD-1 manufacture as a function of the of the number of recycling cycles of the Pd/Al_2O_3 catalyst (C), overall yield (Y) and MIBK/FF molar ratio (R) in the two-reactor process.

Condition	[GWP 100a] (kg CO_2-eq/kg)	Energy (MJ/kg)		Toxicity (kg 1,4-DB-eq/kg)				[Water] (m^3)	[ADP] (kg Sb-eq/kg)	[Land Use] (m^2a/kg)	[AP] (kg SO_2-eq/kg)	[EP] (kg PO_4-eq/kg)	[OLDP] (kg CFC-11-eq/kg)	[POCP] (kg C_2H_4-eq/kg)
		[NRE]	[Renew]	[HTP]	[FAETP]	[MAETP]	[TETP]							
Y=84%, R=18.2, C=3	6.560	120	-	2.211	1.710	1.646	0.1076	0.151	0.0570	1.650	0.0440	0.0120	$8.800x10^{-7}$	$2.400x10^{-3}$
Y=84%, R=18.2, C=30	7.808	128	-	3.030	3.498	2.692	0.5200	0.207	0.0613	1.668	0.0890	0.0169	$9.994x10^{-7}$	$4.533x10^{-3}$
Y=84%, R=18.2, C=300	19.98	212	-	11.17	21.29	13.03	4.649	0.764	0.1036	1.846	0.543	0.0653	$2.159x10^{-6}$	$2.570x10^{-2}$
Y=100%, R=18.2, C=3	5.214	119	-	1.811	1.349	1.266	0.1076	0.151	0.0473	1.383	0.0364	0.0097	$7.052x10^{-7}$	$1.856x10^{-3}$
Y=100%, R=16.2, C=3	5.118	108	-	1.801	1.349	1.265	0.0902	0.126	0.0464	1.383	0.0364	0.0097	$6.948x10^{-7}$	$1.851x10^{-3}$
Y=100%, R=14.2, C=3	5.010	98	-	1.789	1.348	1.263	0.0901	0.126	0.0454	1.383	0.0363	0.0097	$6.833x10^{-7}$	$1.845x10^{-3}$
Y=100%, R=12.2, C=3	4.914	87	-	1.779	1.347	1.261	0.0901	0.126	0.0446	1.382	0.0363	0.0097	$6.730x10^{-7}$	$1.840x10^{-3}$
Y=100%, R=10.2, C=3	4.807	77	-	1.767	1.347	1.260	0.0900	0.126	0.0436	1.382	0.0362	0.0097	$6.614x10^{-7}$	$1.835x10^{-3}$

Table S19. Sensitivity analysis on the benefits of single-reactor towards two-reactor process for the different impact categories for THF-ALD-1 manufacture as a function of the number of recycling cycles of the Pd/Al_2O_3 catalyst (C), overall yield (Y) and MIBK/FF molar ratio (R).

Condition	[GWP 100a] (kg CO_2-eq/kg)	Energy (MJ/kg)		Toxicity (kg 1,4-DB-eq/kg)				[Water] (m^3)	[ADP] (kg Sb-eq/kg)	[Land Use] (m^2a/kg)	[AP] (kg SO_2-eq/kg)	[EP] (kg PO_4-eq/kg)	[OLDP] (kg CFC-11-eq/kg)	[POCP] (kg C_2H_4-eq/kg)
		[NRE]	Renew	[HTP]	[FAETP]	[MAETP]	[TETP]							
Y=86% or 84%, R=18.2, C=3	-0.078	-2.0	-	-0.160	-0.259	-0.174	-0.0505	-0.0097	-0.0020	-0.0292	-0.0090	$-7.932X10^{-6}$	$-1.395X10^{-8}$	$-5.961X10^{-4}$
Y=86% or 84%, R=18.2, C=30	-0.467	-6.0	-	-0.463	-0.927	-0.502	-0.225	-0.0345	-0.0036	-0.0401	-0.0277	$-1.752X10^{-3}$	$-1.624X10^{-9}$	$-1.363X10^{-3}$
Y=86% or 84%, R=18.2, C=300	-4.47	-47	-	-3.54	-7.70	-3.89	-1.97	-0.283	-0.0203	-0.1485	-0.2015	$-1.956X10^{-2}$	$-1.409X10^{-7}$	$-9.232X10^{-3}$
Y=100%, R=18.2, C=3	-0.0015	-0.80	-	-0.137	-0.221	-0.150	-0.0424	-0.0081	-0.0017	-0.0231	-0.0076	$-2.755X10^{-5}$	$-5.803X10^{-9}$	$-5.003X10^{-4}$
Y=100%, R=16.2, C=3	-0.0030	-0.83	-	-0.137	-0.221	-0.150	-0.0424	-0.0081	-0.0017	-0.0231	-0.0076	$-2.814X10^{-5}$	$-7.375X10^{-9}$	$-5.002X10^{-4}$
Y=100%, R=14.2, C=3	-0.0046	-0.87	-	-0.137	-0.221	-0.150	-0.0424	-0.0081	-0.0017	-0.0231	-0.0076	$-2.880X10^{-5}$	$-9.121X10^{-9}$	$-5.001X10^{-4}$
Y=100%, R=12.2, C=3	-0.0060	-0.90	-	-0.137	-0.221	-0.149	-0.0424	-0.0081	-0.0017	-0.0231	-0.0076	$-2.939X10^{-5}$	$-1.070X10^{-9}$	$-5.000X10^{-4}$
Y=100%, R=10.2, C=3	-0.0076	-0.94	-	-0.135	-0.222	-0.149	-0.0424	-0.0082	-0.0017	-0.0232	-0.0076	$-3.005X10^{-5}$	$-1.244X10^{-8}$	$-4.998X10^{-4}$

Definition of Environmental Impacts

GWP (Global Warming Potential) [GWP100]
This indicator reports the potential impact on climate change over a period of 100 years through the emission of greenhouse gases, expressed in kg of CO_2 equivalent (CO_2-eq). It considers greenhouse gas emissions such as carbon dioxide CO_2, methane CH_4, N_2O nitrous oxide, hydrofluorocarbons (HFCs), perfluorocarbons (PFCs) and sulfur hexafluoride all absorbing and infrared emitting gas on the list of the Kyoto Protocol of 1997. This indicator relies on the characterization factors (global warming powers) published by the Intergovernmental Panel for Climate Change (IPCC) in 2013.[S8] The carbon sink, that is the CO_2 of which the carbon is of plant origin, is not considered, so the characterization factor of bio-based methane is modified to consider the CO_2 taken from the atmosphere during its generation.

Toxicity indicators: Human Toxicity [HTP], Freshwater Aquatic Exotoxicity Potential [FAETP], Marine Aquatic Ecotoxicity Potential [MAETP] et Terrestrial Ecotoxicity Potential [TETP]
These indicators measure the impact of carcinogenic and non-carcinogenic compounds, including traces of metallic elements, biocides or organic compounds such as polycyclic aromatic hydrocarbons (PAHs), and fine particles and dioxins on the metabolism of living beings. Factors describing the fate, exposure and effects of toxic substances are defined for an infinite time horizon. For each substance, toxicity is expressed in kg of 1.4-dichlobenzene equivalent (1.4-DB-eq).

Water Use [Water]
The indicator aggregates the amounts of water taken from the natural environment, omitting the amounts used for cooling purposes, and water involved in hydropower production. It considers any local stress factor on the availability of the resource. It is expressed in m^3 of water. Given the high uncertainty related to this indicator, results shall be interpreted with caution.

Energy indicators:
The Primary Energu Demand (PED) is the quantity of energy directly withdrawn from the hydrosphere, atmosphere or geosphere, or energy source without any anthropogenic change. For fossil fuels and uranium, this would be the amount of resource withdrawn expressed in its energy equivalent (i.e. the energy content of the raw material). For renewable resources, the energy involved in biomass consumption is considered. For hydropower, the energy change in potential energy of water (i.e. from the height difference) is considered. The aggregated values of the different energies are defined as follows:

The total **'Primary energy consumption non-renewable' [Non-Renew]**, given in MJ, characterizes the gain from natural gas [gas], crude oil [Oil], coal [Coal] and nuclear [Uranium]. Natural gas and crude oil are used both for energy production and as material constituents (*e.g.*, in plastics). Coal is primarily used for energy production. Uranium is only used for electricity production in nuclear power stations. The total non-renewable energy consumption represents the sum of the 4 previous indicators.

The total **'Primary energy consumption renewable' [Renew]**, given in MJ, comprises hydropower [hydroelectric], wind power [wind], solar energy [solar], geothermic power [geothermal], hydrogen power [hydrogen] and biomass [biomass and forestry]. The end energy (*e.g.*, 1 kWh of electricity) and the primary energy used are not miscalculated with each other; otherwise, the efficiency for production or supply of the end energy is not be accounted for. The total renewable energy consumption represents the sum of the 6 previous indicators.The energy content of manufactured products is considered as feedstock energy content. It is characterized by the net calorific value of the product. It represents the still-usable energy content.

Abiotic Depletion Potential [ADP]
It is the depletion of the environment in terms of mineral resources. The calculation is performed considering the remaining stocks and the current consumption rate of each of the treated mineral resources. The disappearance of living species and the loss of biodiversity associated with certain emissions are not considered by this indicator. Water is not considered in this indicator. It is expressed in kg antimony (Sb) equivalent (Sb) (Sb-eq).

Quantitative Land use [Land Use]
This indicator measures the reduction of biodiversity of species caused by land use. Agriculture and deforestation are major contributors to this category. It is expressed in square metters per year (m^2a).

Acidification Potential [AP]
Acidification is the result of acid rain due to three types of air pollutants: sulfur dioxide, nitrogen oxides and ammonia. These pollutants come mainly from transport and power stations. Various chemical reactions take place in the air that result in the formation of acidic compounds over long distances causing damage to the flora and fauna when they fall on the ground and in the aquatic environment. This indicator for the

CML 2001 method considers terrestrial and aquatic acidification and represents the increase of acidic compounds such as NO_x and SO_x in the atmosphere. It is expressed in kg of SO_2 equivalent (SO_2-eq).

Eutrophication Potential [EP]
Eutrophication is defined as the enrichment of nutrient in aquatic or terrestrial compartments as a result of human intervention. Air pollutants, wastewater and fertilization in agriculture contribute to eutrophication. The result in water is accelerated algae growth, which in turn, prevents sunlight from reaching the lower depths. This leads to a decrease in photosynthesis and less oxygen production. In addition, oxygen is needed for decomposition of dead algae. Both effects decrease the oxygen concentration in water that can lead to fish dying and anaerobic decomposition (decomposition without oxygen). Hydrogen sulphide and methane are thereby produced. The characterization method used (CML) takes account of the emission of nitrogenous and phosphorous substance in air and ground water. It is based on the ability of a substance to contribute to the profusion of algae. It is expressed in kg of phosphate equivalent (PO_4-eq).

Ozone Layer Depletion [DP]
The ozone layer filters out ultraviolet (UV) radiation. This indicator measures the potential reduction of stratospheric ozone layer and thus increases UV radiation reaching the Earth. It has diverse impacts on human health, such as skin cancer and cataracts, and may also damage terrestrial life and aquatic ecosystems. The destruction of the stratospheric ozone layer (particularly over the poles) is mainly due to a catalytic destruction of ozone by atomic chlorine and bromine. The main source of these halogen atoms in the stratosphere is the photodissociation of chlorofluorocarbons (CFCs) such as 'freons' and bromofluorocarbons compounds such as 'halons'. These compounds are transported into the stratosphere after being emitted at the surface of the Earth mainly due to man-made activities. This indicator is expressed in kg of CFC-11 equivalent (CFC11-eq) (CFC = trichlorofluoromethane).

Photochemical Oxidant Creation Potential [POCP]
This indicator measures the effects on human health associated with the formation of tropospheric ozone, also called 'summer smog'. The pollutants that cause ground-level ozone are NO_x and volatile organic compounds (VOCs) that are mainly emitted by road traffic and industry. Under certain clime conditions, these pollutants can react in a complex manner under the influence of solar irradiation and lead to photochemical ozone creation that many be responsible of respiratory disorders. It is expressed in kg of ethylene equivalent (kg C_2H_4-eq).

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