SUPPORTING INFORMATION

Table SI1. The comparison of characterization results of xylenes from Ecoinvent and US LCI by ReCiPe endpoint

Impact category	Unit	US LCI	Ecoinvent
Fossil depletion	kg oil eq	0	0.002391
Metal depletion	kg Fe eq	0	0
Water depletion	m3	0	8.303883
Natural land transformation	m2	0	-8.2E-05
Urban land occupation	m2a	0	0.065173
Agricultural land occupation	m2a	0	0.029242
Ionising radiation	kBq U235 eq	0	0.546267
Marine ecotoxicity	kg 1,4-DB eq	16.56212	1.134174
Freshwater ecotoxicity	kg 1,4-DB eq	16.84403	0.296582
Terrestrial ecotoxicity	kg 1,4-DB eq	0.005545	0.060794
Particulate matter formation	kg PM10 eq	2.025955	1.380628
Photochemical oxidant formation	kg NMVOC	7.00228	4.792205
Human toxicity	kg 1,4-DB eq	2023.5	12.76112
Marine eutrophication	kg N eq	0.202245	0.097999
Freshwater eutrophication	kg P eq	0	0.013282
Terrestrial acidification	kg SO2 eq	7.786484	4.102556
Ozone depletion	kg CFC-11 eq	4.08E-07	3.14E-07

Table SI2. The selection of Pedigree matrix indicator [49]

	Score	Description	Uncertainty factors	Selection
U_1-Reliability	1	Verified data based on measurement	1.00	
	2	Verified data partly based on assumptions or non-verified data based on measurements	1.05	
	3	Non-verified data partly based on qualified estimates	1.10	
	4	Qualified estimate based on data derived from theoretical information	1.20	√
	5	Non-qualified estimate	1.50	
U_2-Completeness	1	Representative data from all sited relevant for the market considered, over an adequate period even out normal fluctuations	1.00	
	2	Representative data from >50% of the sites relevant for the market considered, over an adequate period even out normal fluctuations	1.02	
	3	Representative data from only some sited (≤50%) relevant for the market considered or >50% of sites but from shorter periods	1.05	
	4	Representative data from only one site relevant for the market considered or some sites but from shorter periods	1.10	
	5	Representativeness unknown or data from a small number of sites and from shorter periods	1.20	√
U_3-Temporal correlation	1	Less than 3 years of difference to the time periods of the dataset	1.00	
	2	Less than 6 years of difference of the time period of the dataset	1.03	

	3	Less than 10 years of difference to the time period of the dataset	1.10	√
	4	Less than 15 years of difference to the time period of the dataset	1.20	
	5	Age of data unknown or more than 15 years of difference to the time period of the dataset	1.50	
U_4-Geographical correlation	1	Data from area under study	1.00	
	2	Average data from larger area in which the area under study is included	1.01	
	3	Data from area with similar production conditions	1.02	
	4	Data from area with slightly similar production conidtions		
	5	Data from unknown or distinctly different area	1.10	√
U_5-Furthe technological correlation	1	Data from enterprises, processes and materials under study (i.e. identical technology)	1.00	
	2			
	3	Data on related processes or materials but same technology, OR Data from processes and materials under study but from different technology	1.20	
	4	Data on related processes or materials but different	1.50	

		technology, OR data on laboratory scale processes and same technology		
	5	Data on related processes or materials but on laboratory scale of different technology	2.00	√
U_6-Sample size	1	>100, continous measurement, balance of purchased products	1.00	
	2	>20	1.02	
	3	>10	1.05	
	4	≥3	1.10	
	5	unknown	1.20	√

Table SI3. Heat duty of each unit

	Heat Duty	GJ/ton pX		GJ/ton pX
	Original Flowsheet		Modified Flowsheet	
R1	144.28		144.28	
R2	-178.06		-176.46	
R3	-2.26		-1.83	
R4	-1.92		-0.88	
FL1	33.14		37.84	
FL2	-10.78		-10.82	
FL4	-2.00		-1.66	
FL5			-0.08	
D	-3.66		-5.48	
EVAP	4.41		4.21	
	condenser	reboiler	condenser	reboiler
DC1	-84.73	50.05		
DC2	-15.84	18.63	-15.89	18.25
DC3	-1.22	1.28	-1.47	1.33
DC4	-0.11	0.12	-0.12	0.13
DC5	-6.95	10.13	-3.47	6.69
DC6	-0.72	0.18	-1.18	0.48
Before HEN	Heating	Cooling	Heating	Cooling
	262.23	-308.24	213.21	-219.26
After	Heating	Cooling	Heating	Cooling

HEN				
	112.47	-158.79	68.11	-73.84

1 Negative represents that cooling utility usage