

Table S1 LCI Scenario A: PTA from isobutanol

	Process name input	Amount	Unit
<i>Cultivation phases</i>			
	Sweet corn {GLO} market for sweet corn Cut-off, U	8.9E+02	kg
<i>Isobutanol production</i>			
<u>Input</u>	Water, process, unspecified natural origin/kg	1.2E+03	kg
	Sulfuric acid {RER} production Cut-off, U	6.6E+00	kg
	Sodium hydroxide, without water, in 50% solution state {RER} chlor-alkali electrolysis, membrane cell Cut-off, U	9.9E+00	kg
	Ammonium sulfate, as N {RER} ammonium sulfate production Cut-off, U	2.6E+00	kg
	Phosphate fertiliser, as P2O5 {RER} diammonium phosphate production Cut-off, U	2.6E+00	kg
	Electricity, high voltage {RER} market group for Cut-off, U	3.9E+01	kWh
	Heat, district or industrial, natural gas {Europe without Switzerland} heat production, natural gas, at industrial furnace >100kW Cut-off, U	1.3E+03	MJ
<u>Emission & Waste</u>	Carbon dioxide, biogenic	6.1E+02	kg
	Heat, waste	9.3E+02	MJ
	Treatment, sewage, from residence, to wastewater treatment, class 2/CH U	4.4E-01	m ³
<i>p-Xylene production</i>			
<u>Input</u>	Heat, district or industrial, natural gas {Europe without Switzerland} heat production, natural gas, at industrial furnace >100kW Cut-off, U	8.2E+02	MJ
	Cooling energy {CH} from natural gas, at cogen unit with absorption chiller 100kW Cut-off, U	8.1E+02	MJ
	Electricity, high voltage {RER} market group for Cut-off, U	5.6E+01	MJ
<u>Emission & Waste</u>	Wastewater, average {Europe without Switzerland} treatment of wastewater, average, capacity 1E9l/year Cut-off, U	5.4E+01	kg
<i>Oxidation to PTA</i>			
<u>Input</u>	Oxygen	5.9E+01	kg
	Carbon dioxide, in air	3.5E-01	kg
	Acetic acid, without water, in 98% solution state {RER} acetic acid production, product in 98% solution state Cut-off, U	5.4E-01	kg
	Heat, district or industrial, natural gas {Europe without Switzerland} heat production, natural gas, at industrial furnace >100kW Cut-off, U	6.9E+02	MJ
<u>Emission & Waste</u>	Oxygen	1.5E+00	kg
	Carbon dioxide, biogenic	6.0E-01	kg
	Wastewater, average {Europe without Switzerland} treatment of wastewater, average, capacity 1E9l/year Cut-off, U	2.2E+01	kg

Table S2 LCI Scenario B: PTA from HMF and ethylene

Process name input		Amount	Unit
<i>Bio-ethylene production</i>			
<u>Input</u>	Ethanol, without water, in 95% solution state, from fermentation {RoW} ethanol production from maize Cut-off, U	2.0E+01	kg
	Electricity, high voltage {RER} market group for Cut-off, U	2.1E+01	MJ
	Heavy fuel oil, burned in refinery furnace {Europe without Switzerland} processing Cut-off, U	6.6E+01	MJ
<u>Emission</u>	Methane	1.8E-02	kg
	Carbon monoxide	2.3E-03	kg
	Carbon dioxide	3.8E+00	kg
	NM VOC, non-methane volatile organic compounds, unspecified origin	1.3E-04	kg
	Sulfur dioxide	1.2E-03	kg
	Nitrogen oxides	1.8E-02	kg
	Dinitrogen monoxide	1.4E-04	kg
<i>p-Xylene production</i>			
<u>Input</u>	Sugar, from sugar beet {RoW} beet sugar production Cut-off, U	1.0E+02	kg
	Hydrogen, liquid {RER} chlor-alkali electrolysis, membrane cell Cut-off, U	2.9E+00	kg
	Water, cooling, unspecified natural origin, RER	2.7E+00	m ³
	Electricity, high voltage {RER} market group for Cut-off, U	3.4E+01	MJ
	Steam, in chemical industry {RER} production Cut-off, U	1.0E+03	kg
<u>Emission & Waste</u>	Carbon dioxide	2.3E+00	kg
	Wastewater, average {Europe without Switzerland} treatment of wastewater, average, capacity 1E9l/year Cut-off, U	4.7E+01	kg
<i>Oxidation to PTA</i>			
<u>Input</u>	Oxygen	5.9E+01	kg
	Carbon dioxide, in air	3.5E-01	kg
	Acetic acid, without water, in 98% solution state {RER} acetic acid production, product in 98% solution state Cut-off, U	5.4E-01	kg
	Heat, district or industrial, natural gas {Europe without Switzerland} heat production, natural gas, at industrial furnace >100kW Cut-off, U	6.9E+02	MJ
<u>Emission & Waste</u>	Oxygen	1.5E+00	kg
	Carbon dioxide, biogenic	6.0E-01	kg
	Wastewater, average {Europe without Switzerland} treatment of wastewater, average, capacity 1E9l/year Cut-off, U	2.2E+01	kg

Table S3 LCI Scenario C: PTA from orange peels

	Process name input	Amount	Unit
<i>p-Cymene production</i>			
<u>Input</u>	Orange peels	4.1E+03	kg
	Water, process, unspecified natural origin/kg	4.1E+02	kg
	Electricity, high voltage {RER} market group for Cut-off, U	3.6E+02	kWh
	Steam, in chemical industry {RER} production Cut-off, U	2.3E+02	kg
	Water, cooling, unspecified natural origin, RER	5.2E+01	m ³
<u>Waste</u>	Wastewater, average {Europe without Switzerland} treatment of wastewater, average, capacity 1E9l/year APOS, U	3.5E+03	kg
<u>Avoided product</u>	Composting of wastes	1.7E+04	kg
<i>Oxidation to PTA</i>			
<u>Input</u>	Oxygen	1.7E+01	kg
	Heat, district or industrial, natural gas {Europe without Switzerland} heat production, natural gas, at industrial furnace >100kW Cut-off, U	5.1E+01	MJ
	Cooling energy {CH} from natural gas, at cogen unit with absorption chiller 100kW Cut-off, U	3.3E+02	MJ
	Electricity, high voltage {RER} market group for Cut-off, U	4.8E+01	MJ
<u>Emission & Waste</u>	Wastewater, average {Europe without Switzerland} treatment of wastewater, average, capacity 1E9l/year Cut-off, U	7.3E+00	kg

Table S4 LCI Scenario D: PTA from crude oil

	Process name input	Amount	Unit
<i>PTA production</i>			
<u>Input</u>	Water, cooling, unspecified natural origin, RER	3.4E-01	m ³
	Acetic acid, without water, in 98% solution state {GLO} market for Cut-off, U	5.0E+01	kg
	Chemical factory, organics {GLO} market for Cut-off, U	4.0E-07	p
	Electricity, medium voltage {RER} market group for Cut-off, U	4.7E+02	kWh
	Heat, district or industrial, natural gas {RER} market group for Cut-off, U	4.6E+02	MJ
	Heat, district or industrial, other than natural gas {RER} market group for Cut-off, U	1.2E+03	MJ
	Nitrogen, liquid {RER} market for Cut-off, U	4.9E+01	kg
	Sodium hydroxide, without water, in 50% solution state {GLO} market for Cut-off, U	1.5E+00	kg
	Steam, in chemical industry {GLO} market for Cut-off, U	6.4E+02	kg
	Water, completely softened, from decarbonised water, at user {GLO} market for Cut-off, U	4.3E+02	kg
	Xylene {GLO} market for Cut-off, U	6.6E+02	kg
<u>Emission & Waste</u>	Hydrocarbons, aromatic	0.378	kg
	NMVOC, non-methane volatile organic compounds, unspecified origin	0.11	kg
	Particulates, < 2.5 um	0.02	kg
	Particulates, > 10 um	0.03	kg
	Particulates, > 2.5 um, and < 10um	0.04	kg
	Water/m3	0.22	m ³
	Average incineration residue {GLO} market for Cut-off, U	6.00	kg
	Hazardous waste, for underground deposit {GLO} market for Cut-off, U	0.20	kg

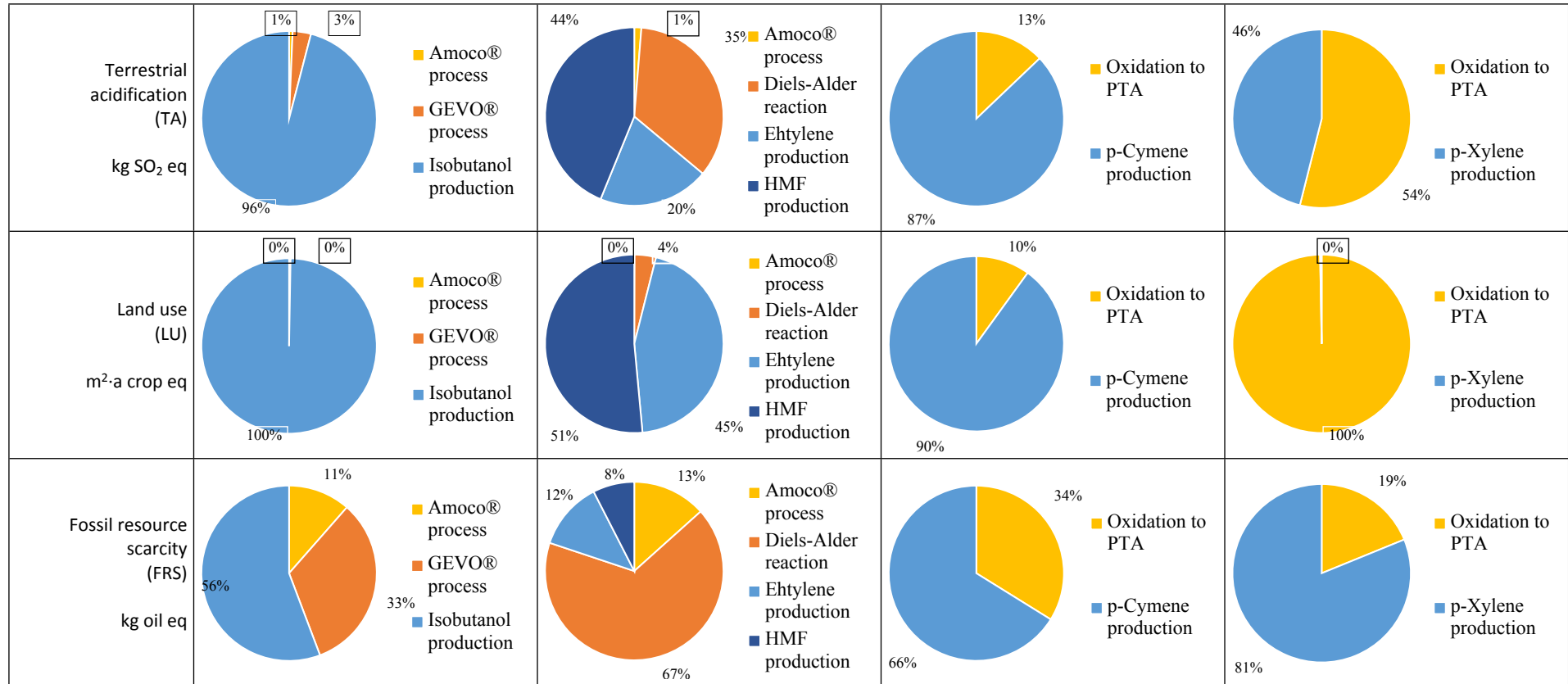
Table S5 Contribution analysis of the midpoint impacts of the scenarios (Cut-off >2%).

		Global warming kg CO ₂ eq	Fine particulate matter formation kg PM2.5 eq	Human toxicity kg 1,4-DCB	Water consumption m ³	Terrestrial acidification kg SO ₂ eq	Land use m ² ·a crop eq	Fossil resource scarcity kg oil eq
Scenario A	Total	5.8E+03	9.4E+00	2.5E+03	4.2E+02	4.3E+01	2.0E+03	1.7E+03
<i>Amoco® process</i>	Heat, district or industrial, natural gas {Europe without Switzerland} heat production, natural gas, at industrial furnace >100kW Cut-off, U	4.9E+02	8.6E-02	1.4E+01	1.5E-01	2.5E-01	3.1E-01	1.9E+02
<i>GEVO® process</i>	Cooling energy {CH} from natural gas, at cogen unit with absorption chiller 100kW Cut-off, U	9.2E+02	3.0E-01	4.8E+02	6.5E+00	8.7E-01	2.5E+00	3.2E+02
	Heat, district or industrial, natural gas {Europe without Switzerland} heat production, natural gas, at industrial furnace >100kW Cut-off, U	5.6E+02	9.9E-02	1.6E+01	1.7E-01	2.9E-01	3.5E-01	2.2E+02
<i>Isobutanol production</i>	Sweet corn {GLO} market for sweet corn Cut-off, U	2.6E+03	7.9E+00	1.5E+03	4.0E+02	3.9E+01	2.0E+03	5.0E+02
	Phosphate fertiliser, as P2O5 {RER} diammonium phosphate production Cut-off, U	3.8E+01	1.4E-01	8.9E+01	2.4E+00	3.7E-01	7.8E+00	1.7E+01
	Sulfuric acid {RER} production Cut-off, U	6.9E+00	1.3E-01	2.6E+01	1.7E+00	4.3E-01	3.1E-01	9.8E+00
	Sodium hydroxide, without water, in 50% solution state {RER} chlor-alkali electrolysis, membrane cell Cut-off, U	7.9E+01	1.5E-01	1.2E+02	2.8E+00	3.7E-01	3.0E+00	1.9E+01
	Ammonium sulfate, as N {RER} ammonium sulfate production Cut-off, U	5.3E+01	5.7E-02	7.5E+01	1.9E-01	1.4E-01	2.1E+00	1.7E+01
	Heat, district or industrial, natural gas {Europe without Switzerland} heat production, natural gas, at industrial furnace >100kW Cut-off, U	8.7E+02	1.5E-01	2.5E+01	2.7E-01	4.5E-01	5.5E-01	3.4E+02
	Electricity, high voltage {RER} market group for Cut-off, U	1.7E+02	2.7E-01	1.3E+02	2.7E+00	7.5E-01	6.0E+00	4.2E+01
Scenario B	Total	5.0E+03	5.9E+00	1.3E+03	1.9E+02	2.2E+01	1.0E+03	1.5E+03
<i>Amoco® process</i>	Heat, district or industrial, natural gas {Europe without Switzerland} heat production, natural gas, at industrial furnace >100kW Cut-off, U	4.9E+02	8.6E-02	1.4E+01	1.5E-01	2.5E-01	3.1E-01	1.9E+02
<i>Diels-Alder reaction</i>	Steam, in chemical industry {RER} production Cut-off, U	2.8E+03	2.0E+00	3.2E+02	4.0E+00	5.9E+00	2.7E+01	8.8E+02
	Hydrogen, liquid {RER} chlor-alkali electrolysis, membrane cell Cut-off, U	3.3E+02	6.0E-01	4.9E+02	1.1E+01	1.5E+00	1.2E+01	7.9E+01
	Electricity, high voltage {RER} market group for Cut-off, U	4.1E+01	6.5E-02	3.2E+01	6.6E-01	1.8E-01	1.5E+00	1.0E+01
<i>Ethylene production</i>	Heavy fuel oil, burned in refinery furnace {Europe without Switzerland} processing Cut-off, U	5.5E+01	2.0E-01	5.6E+00	1.1E-01	6.2E-01	9.4E-02	1.9E+01
	Maize grain {GLO} market for Cut-off, U	4.0E+02	8.8E-01	1.0E+02	1.1E+02	3.2E+00	4.6E+02	7.4E+01

	Electricity, medium voltage {RER} market group for Cut-off, U	6.1E+01	1.3E-01	2.9E+01	3.7E-01	2.2E-01	6.7E-01	1.4E+01
	Heat, district or industrial, natural gas {RER} market group for Cut-off, U	1.5E+02	3.2E-02	5.1E+00	8.0E-02	9.4E-02	1.0E-01	6.0E+01
<i>HMF production</i>	Sugar beet {RoW} market for sugar beet Cut-off, U	3.0E+02	1.4E+00	6.7E+01	4.5E+01	9.0E+00	5.3E+02	5.0E+01
	Electricity, high voltage {RER} market group for Cut-off, U	1.2E+02	2.6E-01	5.5E+01	7.0E-01	4.1E-01	1.3E+00	2.7E+01
	Transport, tractor and trailer, agricultural {GLO} market for Cut-off, U	1.8E+01	4.3E-02	4.7E+01	8.3E-02	8.2E-02	1.2E+00	4.8E+00
	Tap water {RoW} market for Cut-off, U	2.5E+00	5.2E-03	2.1E+00	4.2E+00	9.5E-03	4.3E-02	6.0E-01
Scenario C	Total	4.7E+01	1.7E+00	-4.6E+03	2.1E+02	5.1E+00	3.2E+01	4.9E+02
<i>Oxidation to PTA</i>	Cooling energy {CH} from natural gas, at cogen unit with absorption chiller 100kW Cut-off, U	3.9E+02	1.3E-01	2.0E+02	2.7E+00	3.7E-01	1.1E+00	1.4E+02
	Electricity, high voltage {RER} market group for Cut-off, U	6.0E+01	9.4E-02	4.7E+01	9.6E-01	2.7E-01	2.1E+00	1.5E+01
	Heat, district or industrial, natural gas {Europe without Switzerland} heat production, natural gas, at industrial furnace >100kW Cut-off, U	3.6E+01	6.4E-03	1.0E+00	1.1E-02	1.9E-02	2.3E-02	1.4E+01
<i>p-Cymene production</i>	Electricity, high voltage {RER} market group for Cut-off, U	6.7E+02	1.1E+00	5.3E+02	1.1E+01	3.0E+00	2.4E+01	1.7E+02
	Water, cooling, unspecified natural origin, RER	2.0E+00	1.0E-02	0.0E+00	2.2E+02	0.0E+00	1.0E-01	1.0E+00
	Avoided composting	-1.4E+03	2.4E-01	-5.4E+03	-1.3E+01	8.1E-01	2.0E+00	6.7E+01
	Steam, in chemical industry {RER} production Cut-off, U	2.8E+02	2.0E-01	3.1E+01	4.0E-01	5.9E-01	2.6E+00	8.7E+01
	Wastewater, average {Europe without Switzerland} treatment of wastewater, average, capacity 1E9l/year Cut-off, U	7.7E+00	1.8E-02	4.4E+01	-1.3E+01	5.7E-02	3.9E-01	1.6E+00
Scenario D	Total	1.9E+03	1.9E+00	1.0E+03	2.7E+01	5.4E+00	2.8E+01	1.2E+03
<i>Oxidation to PTA</i>	Steam, in chemical industry {GLO} market for Cut-off, U	2.1E+02	1.9E-01	3.2E+01	2.5E-01	5.3E-01	1.1E+00	6.1E+01
	Electricity, medium voltage {RER} market group for Cut-off, U	2.1E+02	3.3E-01	1.8E+02	3.4E+00	9.5E-01	7.5E+00	5.3E+01
	Nitrogen, liquid {RER} market for Cut-off, U	1.3E+01	2.0E-02	1.1E+01	6.0E-01	5.6E-02	4.5E-01	3.2E+00
	Acetic acid, without water, in 98% solution state {GLO} market for Cut-off, U	9.2E+01	1.6E-01	7.7E+01	2.3E+00	3.5E-01	1.5E+00	5.3E+01
	Heat, district or industrial, other than natural gas {RER} market group for Cut-off, U	1.1E+02	1.5E-01	2.5E+01	5.8E-01	4.6E-01	9.3E+00	2.9E+01
	Chemical factory, organics {GLO} market for Cut-off, U	6.9E+01	2.2E-01	5.7E+02	5.7E-01	4.8E-01	6.4E+00	1.5E+01
	Xylene {RER} Cut-off, U	1.2E+03	7.8E-01	3.6E+00	1.9E+01	2.4E+00	0.0E+00	9.2E+02

Table S6 Contribution of the phases of the processes on the impacts of the scenarios.

Impact Category	Scenario A	Scenario B	Scenario C	Scenario D
Global warming (GW) kg CO ₂ eq	<ul style="list-style-type: none"> Amoco® process GEVO® process Isobutanol production 	<ul style="list-style-type: none"> Amoco® process Diels-Alder reaction Ehtylene production HMF production 	<ul style="list-style-type: none"> Oxidation to PTA p-Cymene production 	<ul style="list-style-type: none"> Oxidation to PTA p-Xylene production
Fine particular matter formation (FPMF) kg PM2.5 eq	<ul style="list-style-type: none"> Amoco® process GEVO® process Isobutanol production 	<ul style="list-style-type: none"> Amoco® process Diels-Alder reaction Ehtylene production HMF production 	<ul style="list-style-type: none"> Oxidation to PTA p-Cymene production 	<ul style="list-style-type: none"> Oxidation to PTA p-Xylene production
Human toxicity (HT) kg 1,4-DCB	<ul style="list-style-type: none"> Amoco® process GEVO® process Isobutanol production 	<ul style="list-style-type: none"> Amoco® process Diels-Alder reaction Ehtylene production HMF production 	<ul style="list-style-type: none"> Oxidation to PTA p-Cymene production 	<ul style="list-style-type: none"> Oxidation to PTA p-Xylene production
Water consumption (WC) m ³	<ul style="list-style-type: none"> Amoco® process GEVO® process Isobutanol production 	<ul style="list-style-type: none"> Amoco® process Diels-Alder reaction Ehtylene production HMF production 	<ul style="list-style-type: none"> Oxidation to PTA p-Cymene production 	<ul style="list-style-type: none"> Oxidation to PTA p-Xylene production



General legend:

- Final oxidation steps (*Amoco process* and *Oxidation to PTA*)
- Transformations to p-Xylene (*GEVO process* and *Diels-Alder reaction*)
- Raw materials (*Isobutanol, Ethylene, HMF, p-Cymene* and *p-Xylene*)

- Negative impacts
- Positive impacts

Table S7 Comparison between PTA production scenarios in terms of ReCiPe 2016 Endpoint H/A – Characterization analysis

Impact category	Unit	Scenario A	Scenario B	Scenario C	Scenario D
Global warming – Human Health	DALY	$5.42 \cdot 10^{-3}$	$4.65 \cdot 10^{-3}$	$4.37 \cdot 10^{-5}$	$1.78 \cdot 10^{-3}$
Fine particulate matter formation	DALY	$5.90 \cdot 10^{-3}$	$3.70 \cdot 10^{-3}$	$1.10 \cdot 10^{-3}$	$1.23 \cdot 10^{-3}$
Human toxicity	DALY	$9.50 \cdot 10^{-4}$	$5.35 \cdot 10^{-4}$	$-1.39 \cdot 10^{-3}$	$4.70 \cdot 10^{-4}$
Water consumption – Human Health	DALY	$9.73 \cdot 10^{-4}$	$4.29 \cdot 10^{-4}$	$4.69 \cdot 10^{-4}$	$5.97 \cdot 10^{-5}$
Global warming – Terrestrial Ecosystems	species-y r	$1.64 \cdot 10^{-5}$	$1.40 \cdot 10^{-5}$	$1.33 \cdot 10^{-7}$	$5.37 \cdot 10^{-6}$
Terrestrial acidification	species-y r	$9.22 \cdot 10^{-6}$	$4.68 \cdot 10^{-6}$	$1.08 \cdot 10^{-6}$	$1.15 \cdot 10^{-6}$
Land use	species-y r	$1.74 \cdot 10^{-5}$	$9.23 \cdot 10^{-6}$	$2.83 \cdot 10^{-7}$	$2.48 \cdot 10^{-7}$
Water consumption – Terrestrial Ecosystems	species-y r	$5.91 \cdot 10^{-6}$	$2.61 \cdot 10^{-6}$	$2.85 \cdot 10^{-6}$	$3.63 \cdot 10^{-7}$
Fossil resource scarcity	USD2013	$5.79 \cdot 10^2$	$4.73 \cdot 10^2$	$1.27 \cdot 10^2$	$4.42 \cdot 10^2$

Table S8 Comparison between PTA production scenarios in terms of ReCiPe 2016 H/A – Single Score

Impact category	Unit	Scenario A	Scenario B	Scenario C	Scenario D
Total impact	Pt	746.13	558.89	96.58	372.46
Global warming	Pt	143.63	123.20	1.16	47.10
Fine particulate matter formation	Pt	116.94	73.34	21.73	24.42
Human toxicity	Pt	18.83	10.60	-27.53	9.31
Water consumption	Pt	32.35	14.26	15.60	1.99
Terrestrial acidification	Pt	20.39	10.35	2.39	2.55
Land use	Pt	38.58	20.43	0.63	0.55
Fossil resource scarcity	Pt	375.40	306.71	82.60	286.54

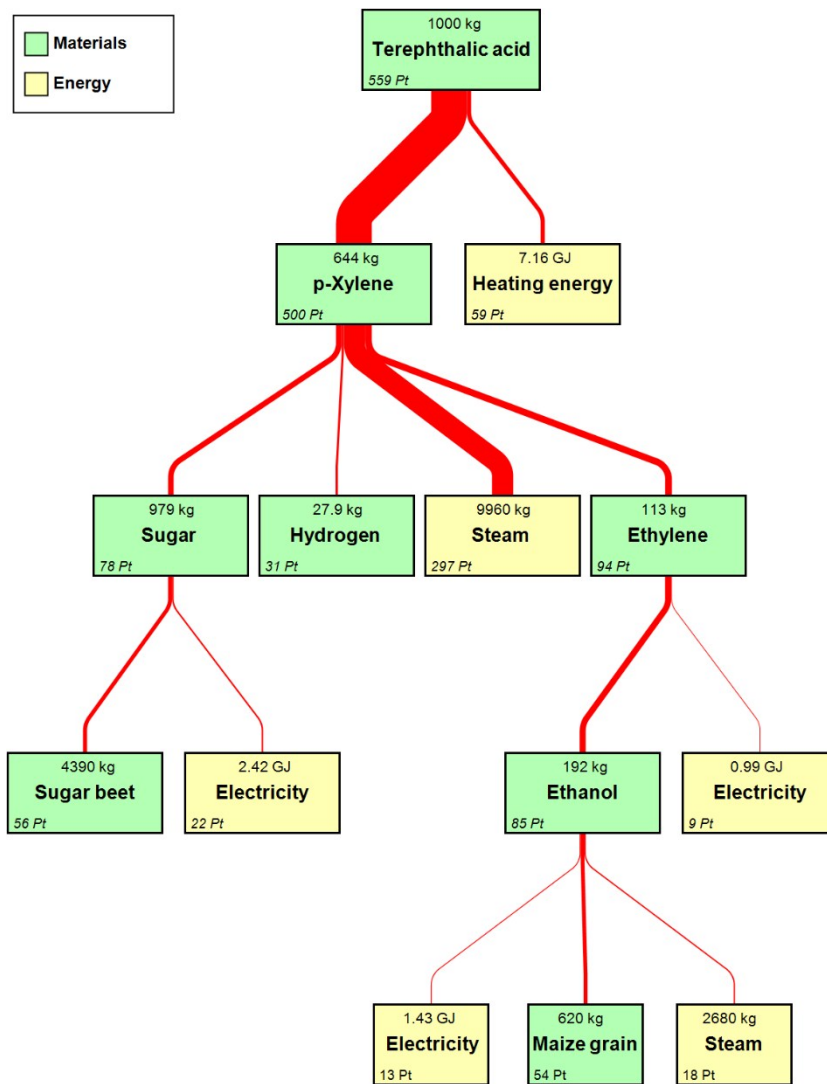


Fig. S1 Contribution analysis for Scenario B (ReCiPe 2016 H/A).

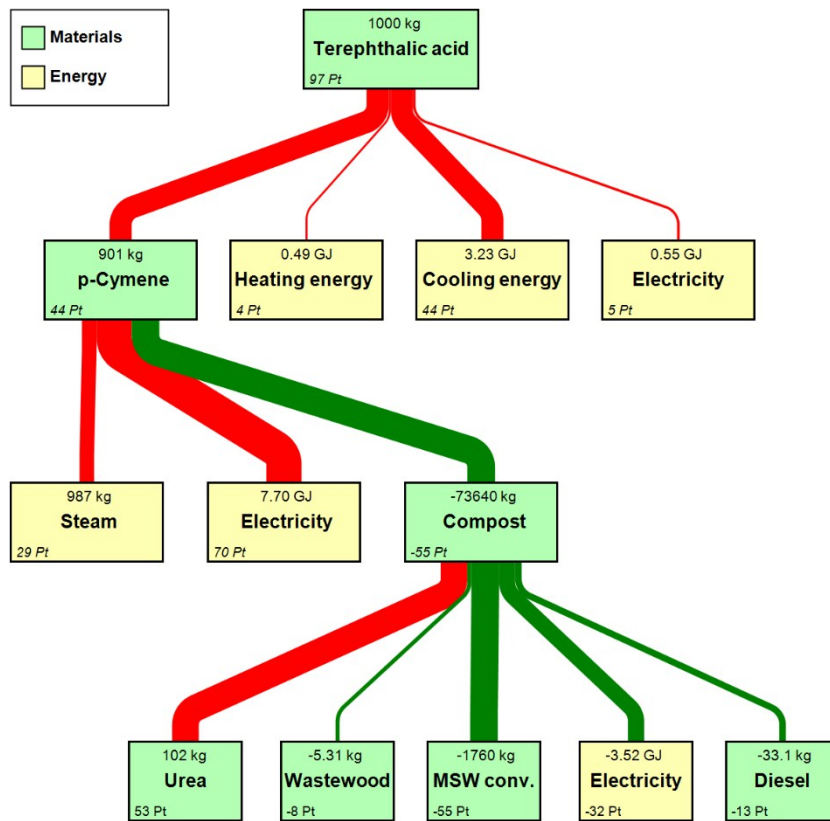


Fig. S2 Contribution analysis for Scenario C (ReCiPe 2016 H/A).

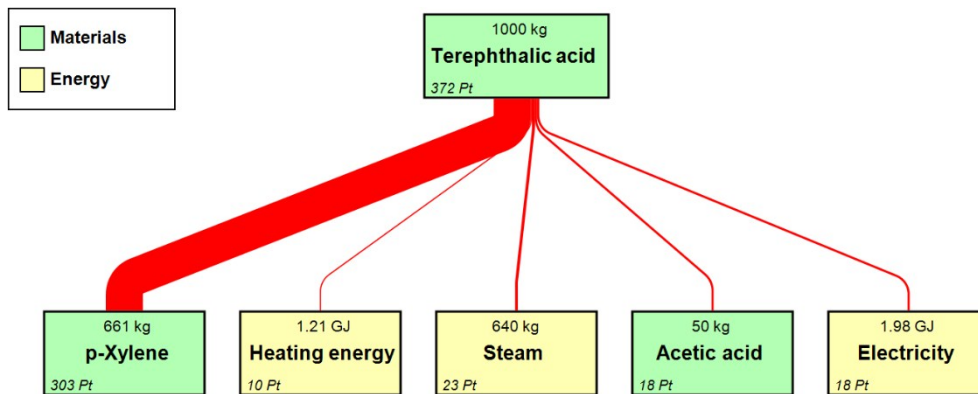


Fig. S3 Contribution analysis for Scenario D (ReCiPe 2016 H/A).

Table S9 Comparison of standard Scenario A and Scenario B with those with 50% waste biomass (ReCiPe 2016 H/A - Single Score).

Impact category	Unit	Scenario A	Scenario A_50%	Difference	Scenario B	Scenario B_50%	Difference
Total impact	Pt	746.13	560.80	- 24.8%	558.89	504.75	- 9.7%
Global warming	Pt	143.63	111.88	- 22.1%	123.20	114.57	- 7.0%
Fine particulate matter formation	Pt	116.94	67.83	- 42.0%	73.34	59.13	- 19.4%
Human toxicity	Pt	18.83	13.13	- 30.3%	10.60	9.64	- 9.1%
Water consumption	Pt	32.35	17.69	- 45.3%	14.26	8.72	- 38.9%
Terrestrial acidification	Pt	20.39	11.20	- 45.1%	10.35	7.48	- 27.7%
Land use	Pt	38.58	19.54	- 49.4%	20.43	10.67	- 47.8%
Fossil resource scarcity	Pt	375.40	319.53	- 14.9%	306.71	294.54	- 4.0%