Supplementary information

Bottlenecks in establishing the environmental impact of bio-based plastics: a case study of bio-based HDPE and bio-based PET

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Biogenic carbon calculations

The amount of biogenic CO_2 stored in 1 kg of bio-HDPE was calculated according to the following equation:

$$m_{BC-HDPE} = \frac{m_{BC}}{m_{HDPE}} \cdot \frac{m_{CO_2}}{m_C} \cdot m_{polymer} = \frac{12.0096}{12.0096 + 2 \cdot 1.00784} \cdot \frac{12.0096 + 2 \cdot 15.99903}{12.0096} \cdot 1 = 3.14\ kg$$

$$m_{BC-part-PET} = \frac{2 \cdot 12.0096}{10 \cdot 12.0096 + 8 \cdot 1.00784 + 4 \cdot 16.00} \cdot \frac{12.0096 + 2 \cdot 15.99903}{12.0096} \cdot 1 = 0.46\ kg$$

$$m_{BC-full-PET} = \frac{10 \cdot 12.0096}{10 \cdot 12.0096 + 8 \cdot 1.00784 + 4 \cdot 16.00} \cdot \frac{12.0096 + 2 \cdot 15.99903}{12.0096} \cdot 1 = 2.29\ kg$$

In this equation, $m_{BCstored}$ is the atmospheric CO_2 stored in the polymer in kg. M_{BC} is the molecular weight of biogenic carbon in 1 repeating unit of the polymer. The molecular structure of polyethylene is $(CH_2)_n$, so it equals the molecular weight of one carbon atom in our case. m_{HDPE} is the molecular weight of one repeating unit of the polymer, m_{CO_2} is the molecular weight of one carbon dioxide molecule, and m_c is the atomic weight of carbon. Finally, $m_{polymer}$ is the mass for which the contained CO_2 is to be calculated, 1 kg in this case. The equation first calculates fraction of the weight of a polymer is biogenic carbon. Every kg polyethylene contains of 0.85 kg of carbon atoms. Next, the relation between CO_2 and atomic carbon is used to compute the weight of the corresponding CO_2, amounting to 3.14 kg for bio-HDPE.

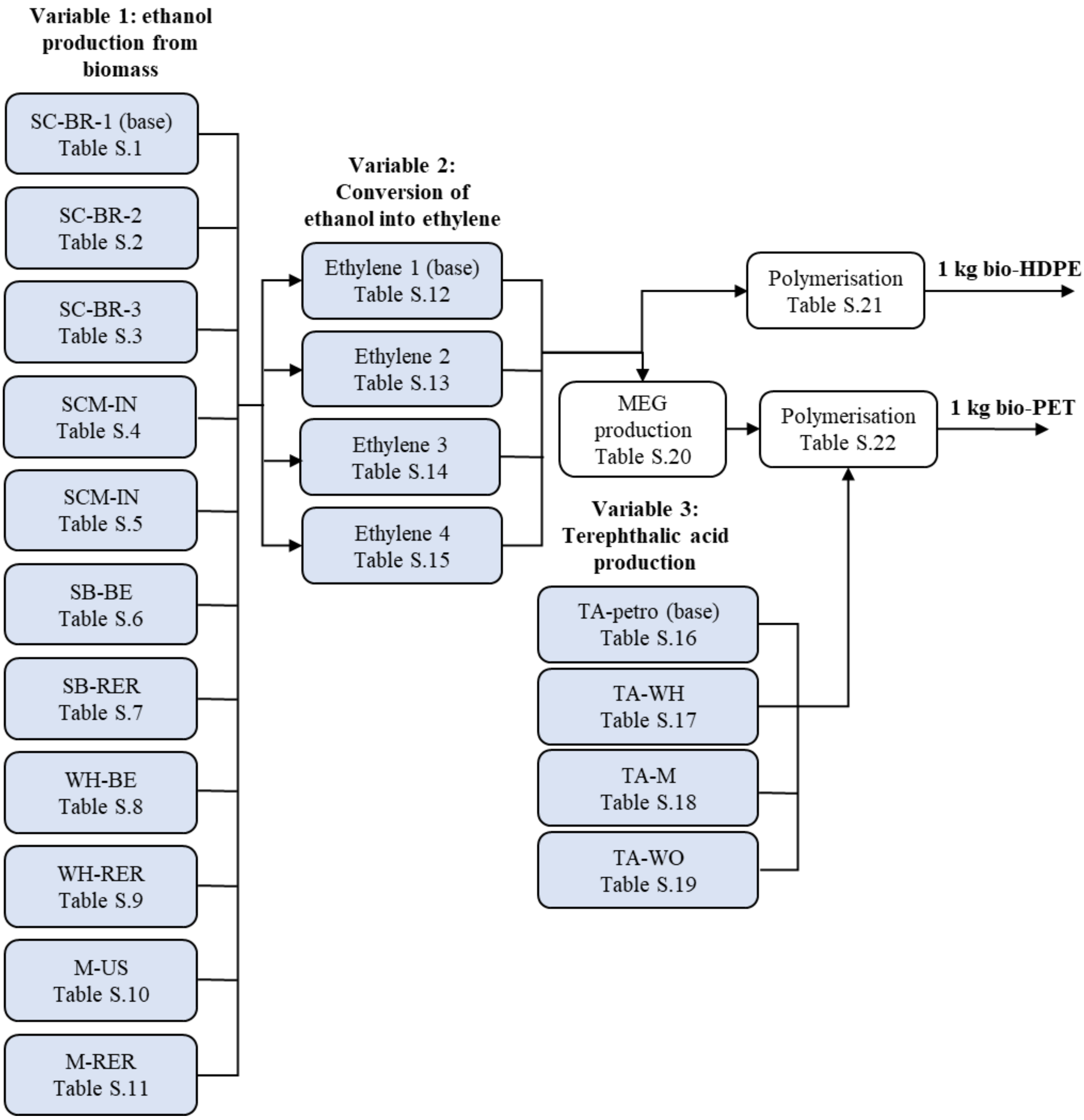


Figure S.1: System diagram for bio-PE and bio-PET, marking the three variables considered in this study and indicating the LCI table with the corresponding scenario.

Table S.1: Lifecycle inventory for SC-BR-1 (base).

Biomass cultivation – 1 kg		
Amount	**Activity**	**Adjustments**
1 kg	Market for sugarcane [BR]	None
Ethanol production – 1 kg		
Amount	**Activity**	**Adjustments**
1 kg	Ethanol, without water, in 99.7% solution state, from fermentation	None

Table S.2: Lifecycle inventory for SC-BR-2.

Biomass cultivation: Sugarcane [BR] – 1000 kg		
Amount	**Activity**	**Adjustments**
147 m^2a	Agricultural land occupation, permanent crop, non-irrigated	
0.11 kg	ammonia, anhydrous, liquid [BR]	
0.29 kg	ammonium nitrate [GLO]	
0.37 kg	Urea [BR]	
0.08 kg	monoammonium phosphate [BR]	
0.146 kg	single superphosphate [RoW]	
0.081 kg	triple superphosphate [BR]	
0.003 kg	phosphate rock, beneficiated [GLO]	
0.022 kg	monoammonium phosphate [BR]	
0.96 kg	potassium chloride [RoW]	
0.01 kg	potassium nitrate [RoW]	
0.01 kg	potassium sulfate [BR]	
0.03901 kg	pesticide, unspecified [RoW]	
0.006 kg	triazine-compound, unspecified [BR]	
0.001 kg	phenoxy-compound [GLO]	
0.002 kg	Glyphosate [RoW]	
5.18 kg	Lime [GLO]	
2.0 kg	hard coal ash [GLO]	
2.3 kg	gypsum, mineral [BR]	
31.0 kg	filter cake, from sugarcane juice filtration [GLO]	
3.6256 kg	Diesel [BR]	
Ethanol production – 1 kg		
Amount	**Activity**	**Adjustments**
14 985 kg	Sugarcane [BR]	
0.15 kg	lubricating oil [RoW]	
13.1 kg	Lime [RoW]	
9.3 kg	sulfuric acid [RoW]	
0.1 kg	pesticide, unspecified [RoW]	
0.86 kg	chemical, organic [GLO]	
24.7 kg	tap water [BR]	
8.32 t km	transport, tractor and trailer, agricultural [RoW]	
-130.0 kg	bagasse, from sugarcane [BR]	
-60.0 kWh	electricity, medium voltage [BR]	

Table S.3: Lifecycle inventory for SC-BR-3.

Biomass cultivation – 1 kg		
Amount	**Activity**	**Adjustments**
1 kg	Market for sugarcane [BR]	None
Ethanol production – 1 kg		
Amount	**Activity**	**Adjustments**
1 kg	Ethanol, without water, in 99.7% solution state, from fermentation	None

Table S.4: Lifecycle inventory for SC-BR-4.

Biomass cultivation: sugarcane [BR] – 25.5 kg		
Amount	**Activity**	**Adjustments**
5.2 MJ	diesel, burned in agricultural machinery [GLO]	
0.0103 kg	chemical, inorganic [GLO]	
147 m^2 a	Agricultural land occupation, permanent crop, non-irrigated	
Ethanol production – 1.7 kg		
Amount	**Activity**	**Adjustments**
12.11 kg	Sugarcane [BR]	
49.5 MJ	Heat, district or industrial, from bagasse [BR]	

Table S.5: Lifecycle inventory for SCM-IN.

Sugarcane production – 1000 kg*		
Amount	**Activity**	**Adjustments**
169 m^2a	Land occupation, permanent crop, irrigated	
59.5 m^3	Irrigation [IN]	
0.42 kg	ammonium sulfate [RoW]	
0.42 kg	ammonium nitrate [RoW]	
0.37 kg	diammonium phosphate [RoW]	
1.23 kg	urea [RoW]	
0.25 kg	potassium nitrate [RoW]	
0.62 kg	diammonium phosphate [RoW]	
0.4 kg	single superphosphate [RoW]	
0.2 kg	triple superphosphate [RoW]	
0.07 kg	phosphate rock, beneficiated [RoW]	
0.8 kg	potassium chloride [RoW]	
0.008 kg	potassium nitrate [RoW]	
0.008 kg	potassium sulfate [RoW]	
0.118 kg	pesticide, unspecified [RoW]	
0.011 kg	triazine-compound, unspecified [RoW]	
0.003 kg	phenoxy-compound [RoW]	
0.004 kg	glyphosate [RoW]	
2.0 kg	hard coal ash [RoW]	
40.0 kg	filter cake, from sugarcane juice filtration [GLO]	
0.5441 kg	Diesel [IN]	
12.0 kWh	electricity, medium voltage [IN]	
Processing into sugarcane molasses – 50.3 kg*		
Amount	**Activity**	**Adjustments**
1000.0 kg	Sugarcane production, from SC-BR-2 [IN]	
1.5 kg	sulfur dioxide, liquid [RoW]	
1.9 kg	limestone, unprocessed [RoW]	
0.5 kg	sodium hydroxide, without water, in 50% solution state [GLO]	
0.1 kg	single superphosphate [RoW]	
0.03 kg	soda ash, dense [GLO]	
0.01 kg	chemical, organic [GLO]	
0.6 kg	lubricating oil [RoW]	
0.01 kg	phosphoric acid, fertiliser grade, without water, in 70% solution state [RoW]	
30.0 kg	tap water [IN]	
12.6 t km	transport, freight train [IN]	

-54.2 kWh	electricity, medium voltage [IN]	
Ethanol production – 1000 kg		
Amount	**Activity**	**Adjustments**
446.08 kg	Sugarcane molasses [IN]	
0.41 kg	sulfuric acid [RoW]	
0.11 kg	magnesium sulfate [RoW]	
1.3 kg	urea [RoW]	
0.14 kg	phosphoric acid, industrial grade, without water, in 85% solution state [RoW]	
0.38 kg	chlorine, liquid [RoW]	
0.06 kg	sodium bicarbonate [RoW]	
0.1 kg	chromium oxide, flakes [RoW]	
0.6 kg	sodium hydroxide, without water, in 50% solution state [GLO]	
0.12 kg	Zinc [GLO]	
0.02 kg	Formaldehyde [RoW]	
11.4 kg	tap water [IN]	
380.0 t km	transport, freight train [IN]	

* Economic allocation was used for the processing of sugarcane, resulting in 8.8% being allocated to sugarcane molasses.

Table S.6: Lifecycle inventory for SB-BE.

Biomass cultivation – 1000 kg*		
Amount	**Activity**	**Adjustments**
1.52 kg	inorganic nitrogen fertiliser, as N [BE]	
2.53 kg	inorganic potassium fertiliser, as K2O [BE]	
1.10 kg	inorganic phosphorus fertiliser, as P2O5 [BE]	
0.04 kg	pesticide, unspecified [RER]	
2.05 kg	Diesel [Europe without Switzerland]	
13.69 m^2a	Land occupation, permanent crop, non-irrigated	
Ethanol production – 783 kg*		
Amount	**Activity**	**Adjustments**
9904 kg	Sugar beet [BE]	
163.0 kWh	electricity, medium voltage [BE]	
6248.0 MJ	heat, district or industrial, natural gas [BE]	
0.3 kg	lubricating oil [RER]	
191.5 kg	lime [RER]	
7.4 kg	sulfuric acid [RER]	
0.25 kg	hydrochloric acid, without water, in 30% solution state [RER]	
10.6 kg	gypsum, mineral [RER]	
0.55 kg	EDTA, ethylenediaminetetraacetic acid [RER]	
0.5 kg	sodium bicarbonate [RER]	

*Using economic allocation, 84% of impacts are allocated to ethanol from sugar beet.

Table S.7: Lifecycle inventory for SB-RER.

Biomass cultivation – 100 kg		
Amount	**Activity**	**Adjustments**
59 kg	Sugar beet production [FR]	
41 kg	Sugar beet production [DE]	
Ethanol production – 1 kg		
Amount	**Activity**	**Adjustments**
11.22	Sugar beet [RER]	
1.03 MJ	heat, from steam, in chemical industry [RER]	
0.00505 kg	ammonia, anhydrous, liquid [RER]	
0.0101 kg	sodium hydroxide, without water, in 50% solution state [GLO]	
0.0193 kg	sulfuric acid [RER]	

Table S.8: Lifecycle inventory for WH-BE.

Biomass cultivation – 1000 kg*		
Amount	**Activity**	**Adjustments**
19.65 kg	inorganic nitrogen fertiliser, as N [BE]	
10.81 kg	inorganic potassium fertiliser, as K2O [BE]	
6.63 kg	inorganic phosphorus fertiliser, as P2O5 [BE]	
0.36 kg	pesticide, unspecified [RER]	
9.19 kg	Diesel [Europe without Switzerland]	
116.28 m^2a	Land occupation	
Ethanol production – 783 kg		
Amount	**Activity**	**Adjustments**
2905 kg	Wheat [BE]	
235.0 kWh	electricity, medium voltage [BE]	
1800.0 MJ	heat, district or industrial, natural gas [BE]	
1.7 kg	sulfuric acid [RER]	
6.65 kg	sodium bicarbonate [RER]	
0.21 kg	magnesium sulfate [RER]	
3.6 kg	ammonia, anhydrous, liquid [RER]	

*Using economic allocation, 67% of impacts are allocated to ethanol from wheat.

Table S.9: Lifecycle inventory for WH-RER.

Biomass cultivation – 100 kg		
Amount	**Activity**	**Adjustments**
41.7 kg	Wheat grain [FR]	
58.3 kg	Wheat grain [DE]	
Ethanol production – 1 kg		
Amount	**Activity**	**Adjustments**
3.73 kg	Wheat [RER]	
13.6 MJ	heat, from steam, in chemical industry [RER]	
0.64 kWh	electricity, medium voltage [RER]	
0.0101 kg	sodium hydroxide, without water, in 50% solution state [GLO]	
0.00505 kg	ammonia, anhydrous, liquid [RER]	
0.0193 kg	sulfuric acid [RER]	

Table S.10: Lifecycle inventory for M-RER.

Biomass cultivation – 1 kg		
Amount	**Activity**	**Adjustments**
1 kg	Maize grain, feed, Swiss integrated production [CH]	
Ethanol production – 1 kg		
Amount	**Activity**	**Adjustments**
2.55 kg	Maize [RER]	
11.85 MJ	heat, from steam, in chemical industry [RER]	
0.27 kWh	electricity, medium voltage [RER]	
0.0061 kg	ammonia, anhydrous, liquid [RER]	
0.0101 kg	sodium hydroxide, without water, in 50% solution state [GLO]	
0.0027 kg	quicklime, milled, packed [RER]	
0.0033 kg	sulfuric acid [RER]	
0.0011 kg	urea [RER]	

Table S.11: Lifecycle inventory for M-US.

Biomass cultivation – 1 kg		
Amount	**Activity**	**Adjustments**
1 kg	Maize grain production [US]	
Ethanol production – 1 kg		
Amount	**Activity**	**Adjustments**
1 kg	ethanol, without water, in 99.7% solution state, from fermentation [US]	

Table S.12: Lifecycle inventory for ethylene 1 (base).

Ethylene production – 1kg		
Amount	**Activity**	**Adjustments**
2.08 kg	Ethanol	
0.1044 kg	nitrogen, liquid [RoW]	
0.11 kg	zeolite, powder [RoW]	
0.0266 kg	sodium bicarbonate [RoW]	
2.57 kg	tap water [BR]	
0.0035 kg	Propylene [RoW]	
0.47 kWh	electricity, medium voltage [BR]	
4.84 MJ	heat, district or industrial, from Bagasse [BR]	

Table S.13: Lifecycle inventory for ethylene 2.

Ethylene production – 783 kg		
Amount	**Activity**	**Adjustments**
1.06 kg	Ethanol	
1210 kg	steam, in chemical industry [RER]	
340 kWh	electricity, medium voltage [BE]	
200 MJ	heat, district or industrial, natural gas [BE]	

Table S.14: Lifecycle inventory for ethylene 3.

Ethylene production – 1kg		
Amount	**Activity**	**Adjustments**
1.70 kg	Ethanol	
5.6 MJ	heat, district or industrial, other than natural gas, Bagasse [BR]	
0.5 kWh	electricity, medium voltage [BR]	

Table S.15: Lifecycle inventory for ethylene 4.

Ethylene production – 1kg		
Amount	**Activity**	**Adjustments**
1.65 kg	Ethanol	
0.32 kWh	electricity, medium voltage [US]	
Polymerisation – 1kg		
Amount	**Activity**	**Adjustments**
1 kg	Polyethylene, high density, granulate [RoW]	Replacing petrochemical ethylene with bio-based ethylene, using the Brazilian market for electricity

Table S.17: Lifecycle inventory for TA-petro (base).

Terephthalic acid production – 1 kg		
1 kg	Purified terephthalic acid	Adjusted for the region of production

Table S.17: Lifecycle inventory for TA-WH.

Terephthalic acid production – 1 kg		
0.000342 kg	tap water [RoW]	
1.012 kg	cyclohexa-2,5-diene-1,4-dicarboxylate [US]	
0.425 kg	water, completely softened [US]	
0.05 kg	acetic acid, without water, in 98% solution state [RoW]	
0.096 kg	oxygen, liquid [RoW]	
0.0488 kg	nitrogen, liquid [RoW]	
0.469 kWh	electricity, medium voltage [US]	
0.637 MJ	heat, district or industrial, other than natural gas [RoW]	
0.212 MJ	heat, district or industrial, other than natural gas [RoW]	
0.323 MJ	heat, district or industrial, natural gas [RoW]	
0.64 kg	steam, in chemical industry [RoW]	

Table S.18: Lifecycle inventory for TA-M.

Iso-butanol production – 1 kg		
4.013 kg	maize grain [US]	
5.255 kg	tap water [RoW]	
0.3 kg	sulfuric acid [RoW]	
0.045 kg	sodium bicarbonate [RoW]	
0.012 kg	ammonium sulfate [RoW]	
0.012 kg	diammonium phosphate [RoW]	
1.60 MJ	heat, district or industrial, natural gas [RoW]	
0.178 kWh	electricity, medium voltage [US]	
Iso-butylene production – 1 kg		
1.32 kg	Isobutanol	
0.5 kWh	electricity, medium voltage [US]	
5.6 MJ	heat, district or industrial, natural gas [RoW]	
Iso-octene production – 1 kg		
2.0 kg	steam, in chemical industry [RoW]	
0.0014 kg	oxygen, liquid [RoW]	
0.0024 kg	tap water [RoW]	
1.0 kg	Iso-butylene	
Iso-octane production – 1 kg		
0.982 kg	Isooctene	
0.048 kWh	electricity, medium voltage [US]	
0.283 MJ	heat, district or industrial, natural gas [RoW]	
0.018 kg	hydrogen, liquid [RoW]	
Para-xylene production – 1 kg		
0.029 kWh	electricity, medium voltage [US]	
2.52 MJ	heat, district or industrial, natural gas [RoW]	
1.08 kg	isooctane	
Terephthalic acid production – 1 kg		
1 kg	Purified terephthalic acid production [RoW]	Replacing petrochemical-based para-xylene with bio-based para-xylene

Table S.19: Lifecycle inventory for TA-WO.

Wood feedstock handling – 907.19 kg		
996.86 kg	Softwood Forest Residues at Gate [US]	
20.95 kg	electricity, medium voltage [US]	
Softwood production – 907.19 kg*		
645.34 kg	Softwood feedstock accepts [US]	
13.94 kg	limestone, crushed, washed [RoW]	
1360.0 kg	water, decarbonised [US]	
334.92 kg	steam, in chemical industry [RoW]	
13.94 kg	Sulphur [RoW]	
6.98 kWh	electricity, medium voltage [US]	
Enzymatic hydrolysis into hydrolysate – 907.19 kg		
426.51 kg	Pulp feed [US]	
0.58 kg	Enzymes [RoW]	
7.45 kg	Glucose [GLO]	
1.03 kg	quicklime, in pieces, loose [RoW]	

0.04 kg	ammonia, anhydrous, liquid [RoW]	
449.21 kg	water, decarbonised [US]	
0.97 kg	steam, in chemical industry [RoW]	
0.38 kWh	electricity, medium voltage [US]	
Isobutanol production – 907.19 kg		
17335.28 kg	Hydrolysate [US]	
34.75 kg	water, decarbonised [US]	
2968.93 kg	steam, in chemical industry [RoW]	
3081.17 kg	electricity, medium voltage [US]	
Para-xylene production – 907.19 kg		
2399.98 kg	Isobutanol	
59.02 kg	water, decarbonised [US]	
20.73 kg	hydrogen, gaseous [RoW]	
491.02 kg	steam, in chemical industry [RoW]	
812.11 kWh	electricity, medium voltage [US]	
Terephthalic acid production – 1 kg		
1 kg	Purified terephthalic acid production [RoW]	Replacing petrochemical-based para-xylene with bio-based para-xylene

Table S.20: Lifecycle inventory for bio-MEG production.

Ethylene oxide production – 1 kg		
1 kg	Ethylene oxide [RoW]	Replacing petrochemical ethylene with bio-based ethylene, using the local market for electricity
Monoethylene glycol production – 1 kg		
1 kg	Ethylene glycol [RoW]	Replacing petrochemical ethylene with bio-based ethylene, using the local market for electricity

Table S.21: Lifecycle inventory for bio-HDPE production.

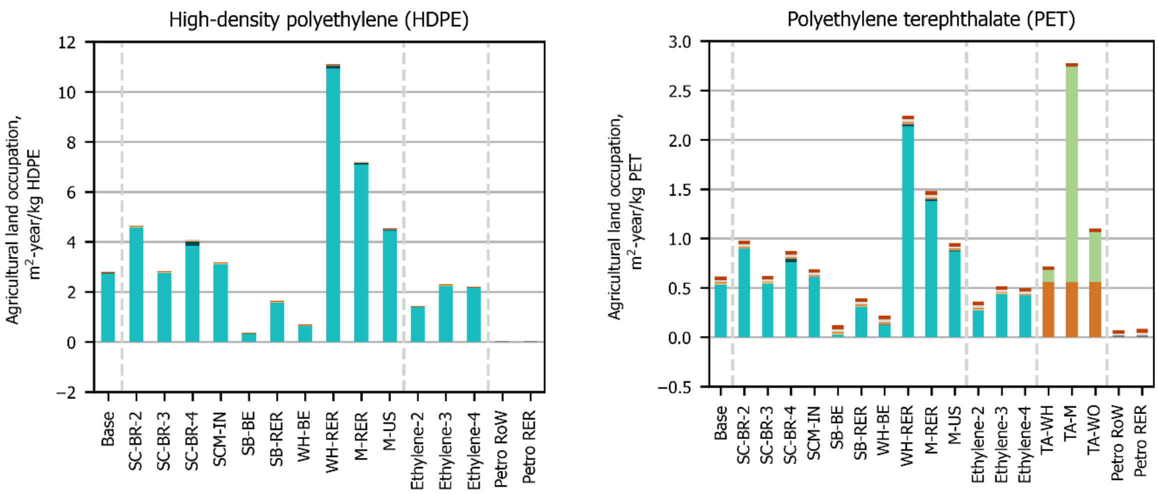
Polymerisation – 1 kg		
Amount	**Activity**	**Adjustments**
1 kg	Polyethylene, high density, granulate [RER or RoW]	Replacing petrochemical ethylene with bio-based ethylene, adjusting the location.

Table S.22: Lifecycle inventory for bio-PET production.

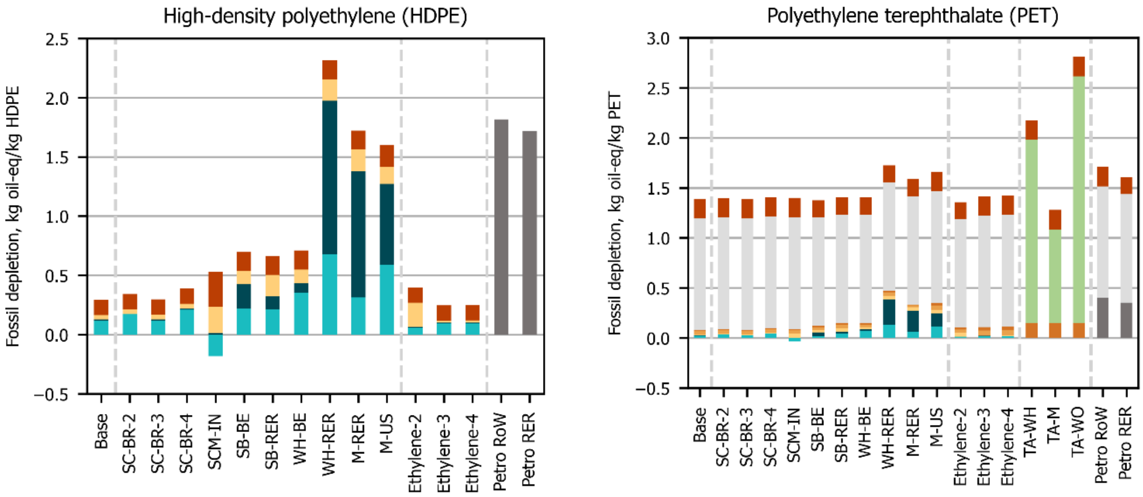
Polymerisation – 1 kg		
Amount	**Activity**	**Adjustments**
1 kg	polyethylene terephthalate, granulate, amorphous [RER]	Replacing petrochemical MEG and TA with bio-based MEG/TA and adjusting the location.

Table S.23: Outcomes ReCiPe end-point environmental impact.

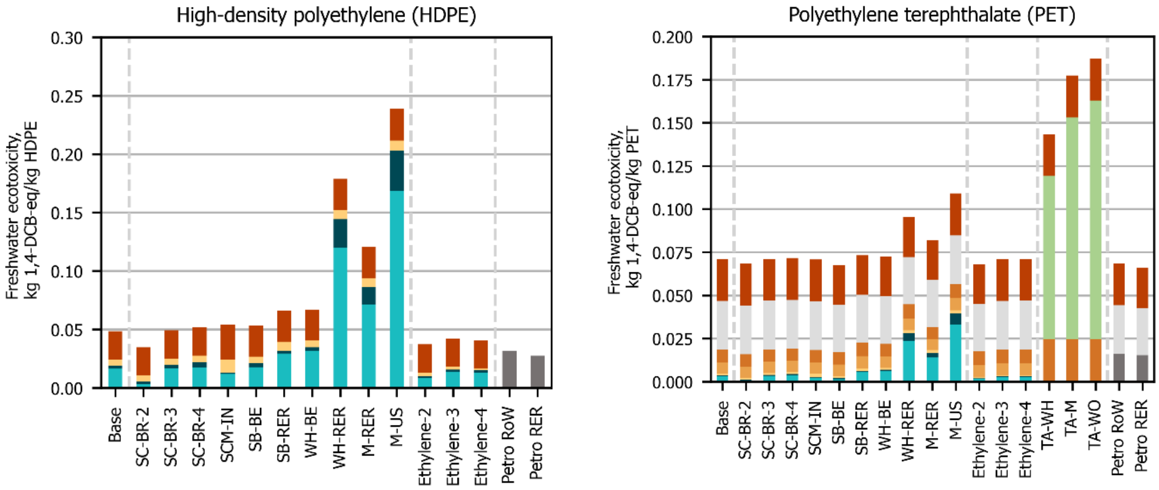
Environmental impact category	**Outcome (points)**
ReCiPe Endpoint (H,A) | ecosystem quality | agricultural land occupation	0.079122
ReCiPe Endpoint (H,A) | ecosystem quality | climate change, ecosystems	0.027427
ReCiPe Endpoint (H,A) | ecosystem quality | freshwater ecotoxicity	3.35E-05
ReCiPe Endpoint (H,A) | ecosystem quality | freshwater eutrophication	3.37E-05
ReCiPe Endpoint (H,A) | ecosystem quality | marine ecotoxicity	3.88E-06
ReCiPe Endpoint (H,A) | ecosystem quality | natural land transformation	0.007504
ReCiPe Endpoint (H,A) | ecosystem quality | terrestrial acidification	0.000424
ReCiPe Endpoint (H,A) | ecosystem quality | terrestrial ecotoxicity	6.75E-05
ReCiPe Endpoint (H,A) | ecosystem quality | urban land occupation	0.001007
ReCiPe Endpoint (H,A) | human health | climate change, human health	0.043392
ReCiPe Endpoint (H,A) | human health | human toxicity	0.00775
ReCiPe Endpoint (H,A) | human health | ionising radiation	1.72E-05
ReCiPe Endpoint (H,A) | human health | ozone depletion	3.22E-06
ReCiPe Endpoint (H,A) | human health | particulate matter formation	0.095971
ReCiPe Endpoint (H,A) | human health | photochemical oxidant formation	0.001625
ReCiPe Endpoint (H,A) | resources | fossil depletion	0.03534
ReCiPe Endpoint (H,A) | resources | metal depletion	0.011642



(a) Agricultural land occupation.

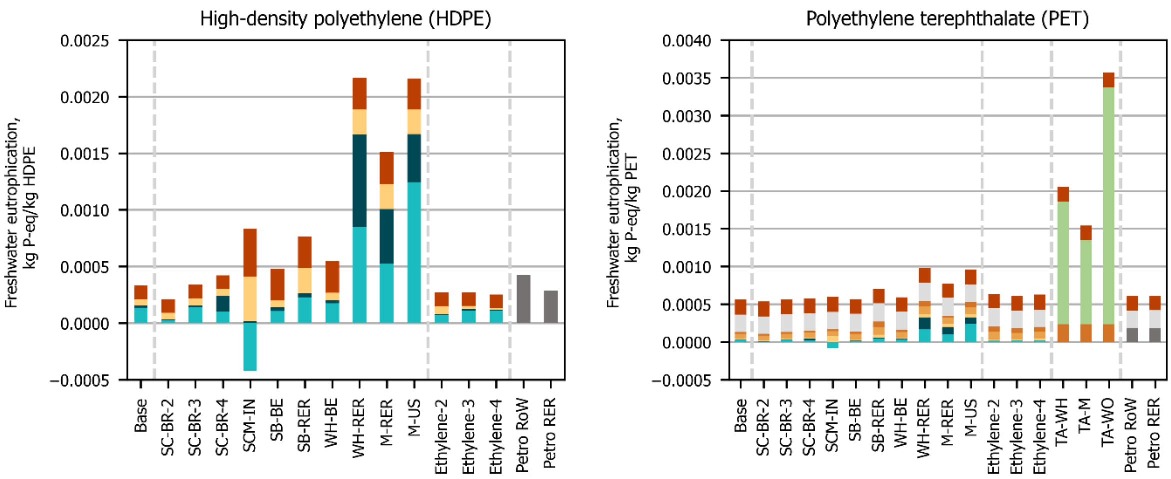


(b) Fossil depletion.

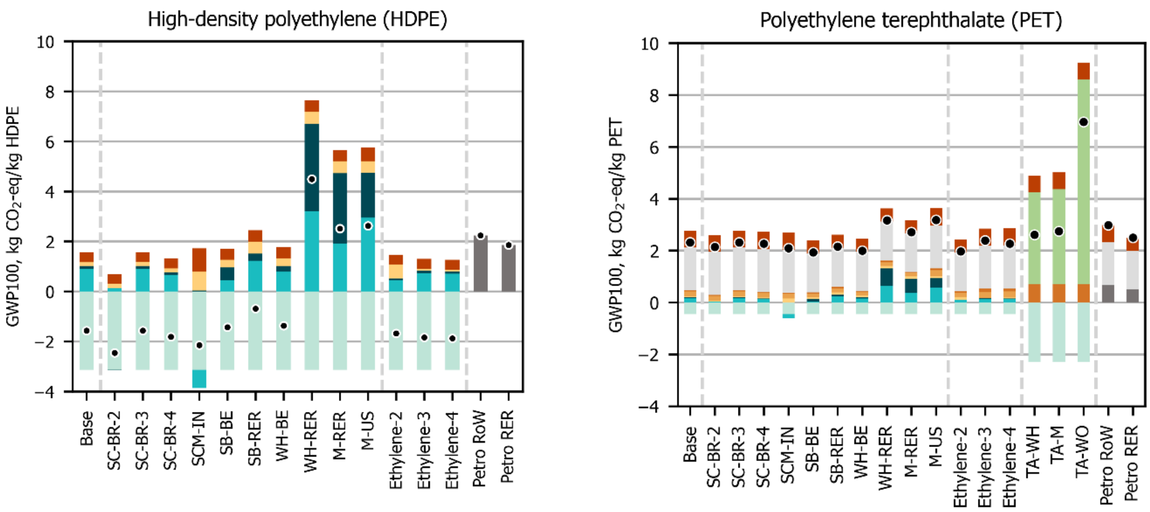


(c) Freshwater ecotoxicity.

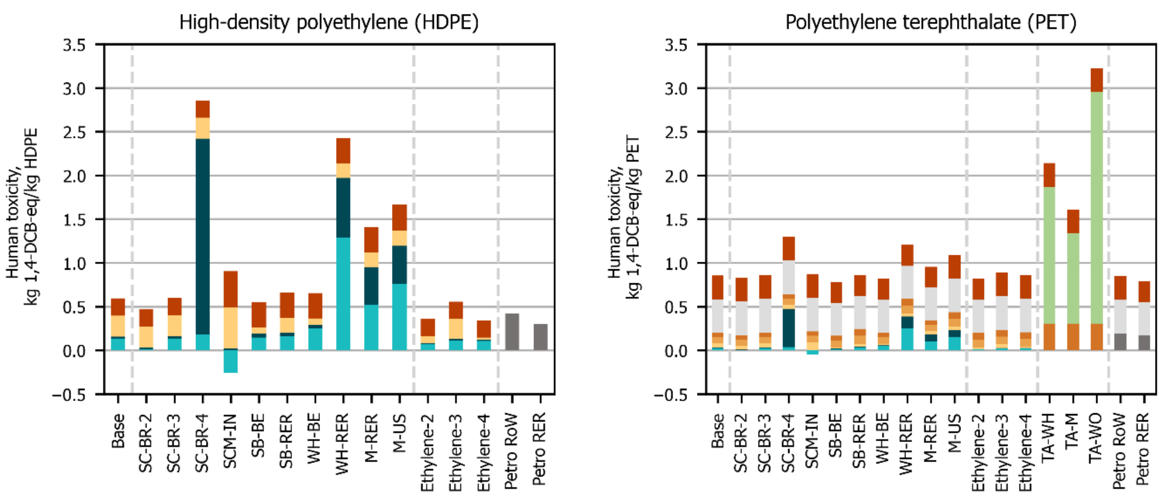
Figure S.2: Environmental impact of bio-based and petrochemical-based HDPE and PET.



(d) Freshwater eutrophication.



(e) Global warming potential (GWP100).



(f) Human toxicity.

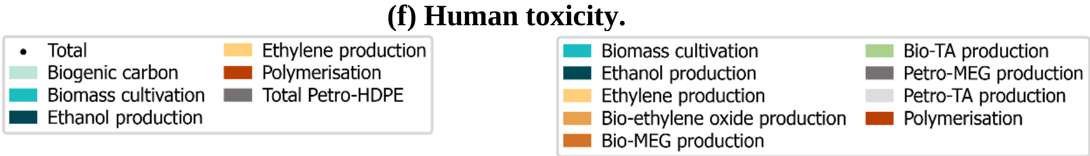
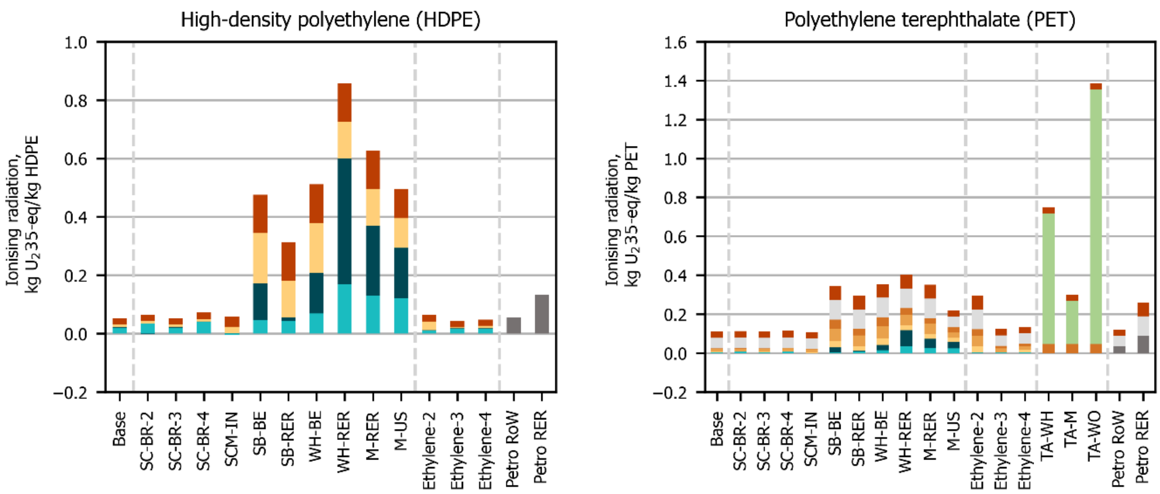
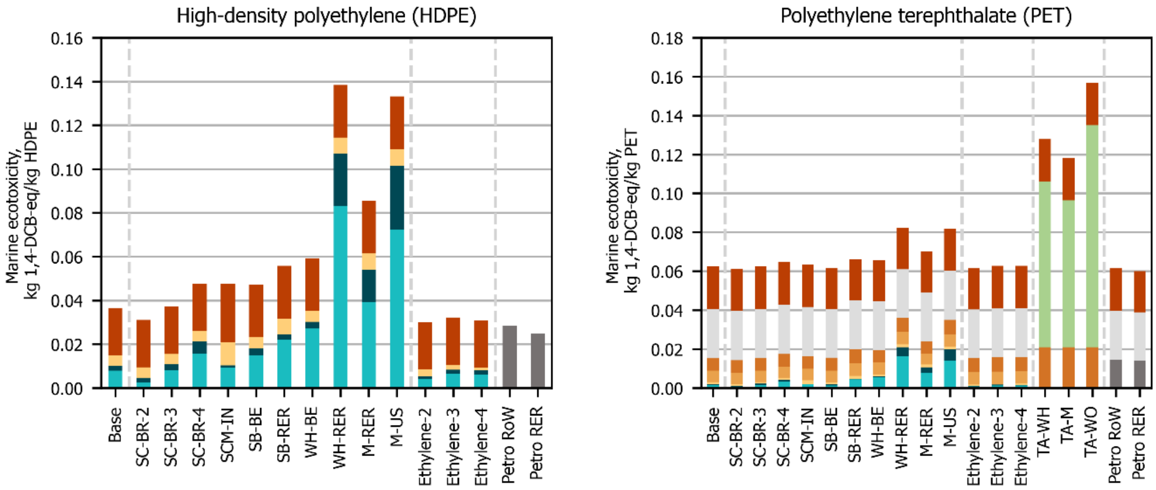


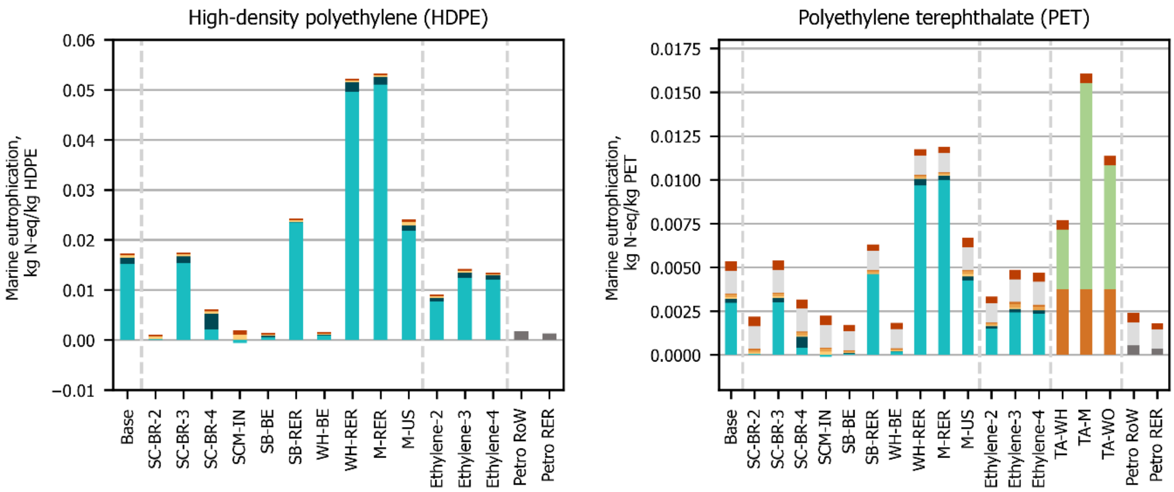
Figure S.2 continued.



(g) **Ionising radiation.**

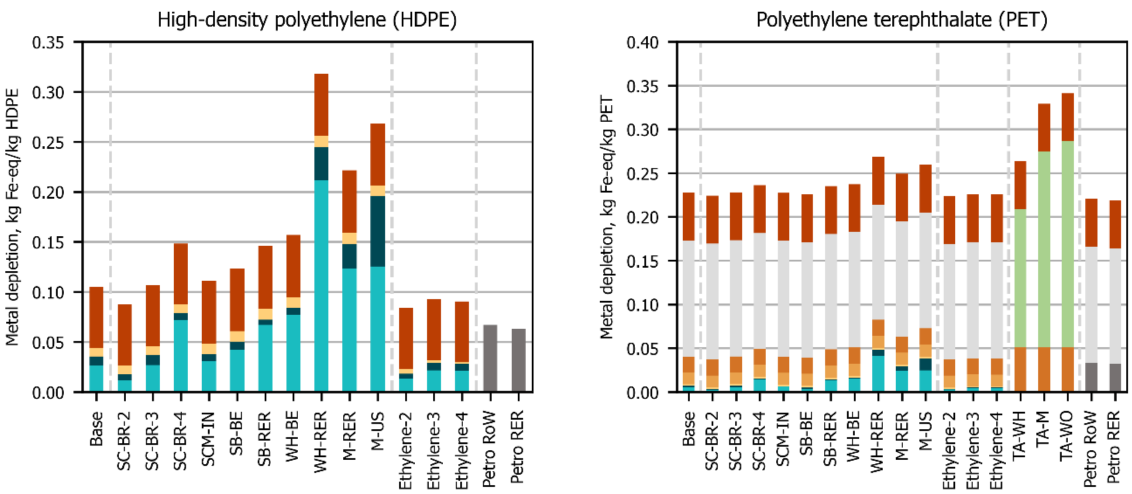


(h) **Marine ecotoxicity.**

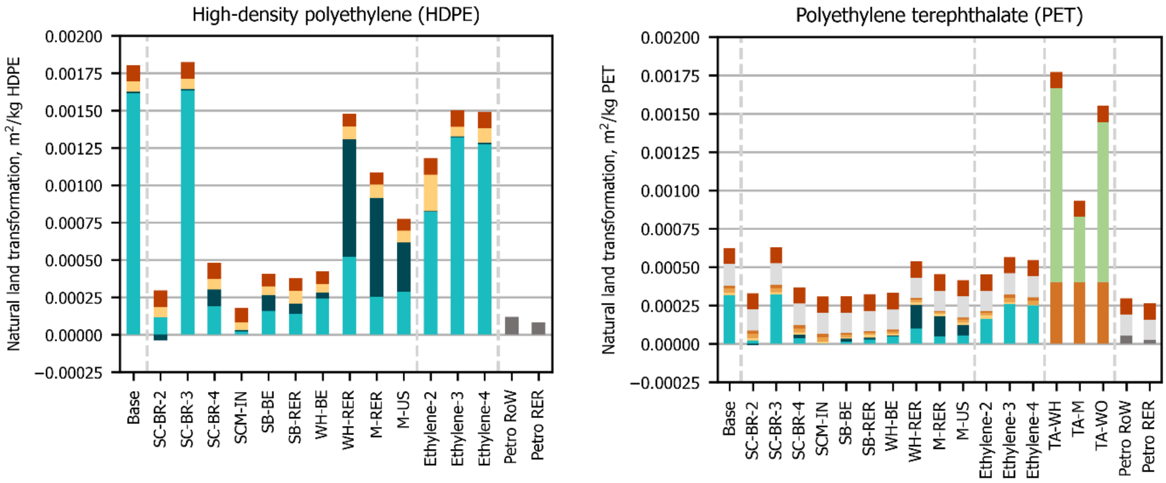


(i) **Marine eutrophication.**

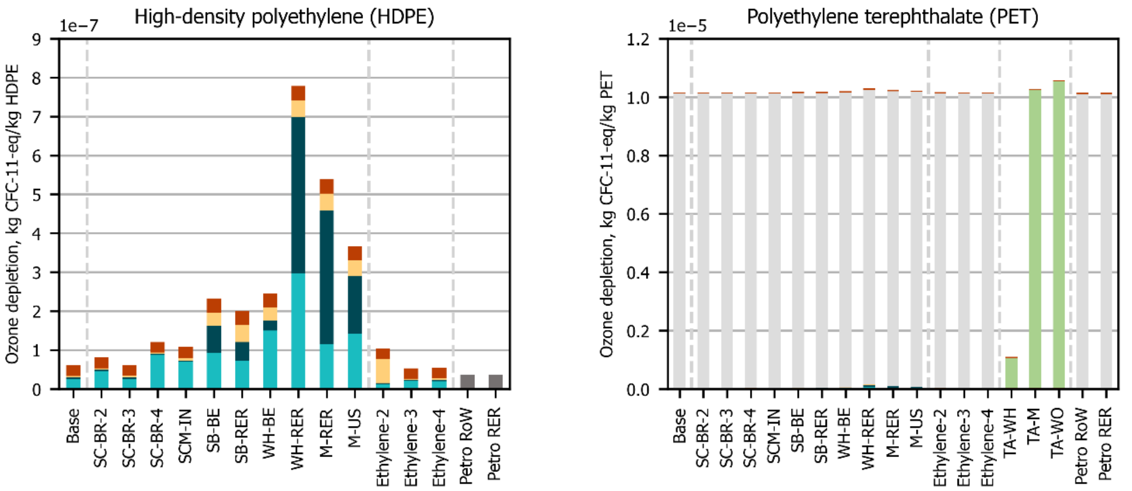
Figure S.2 continued.



(j) Metal depletion.

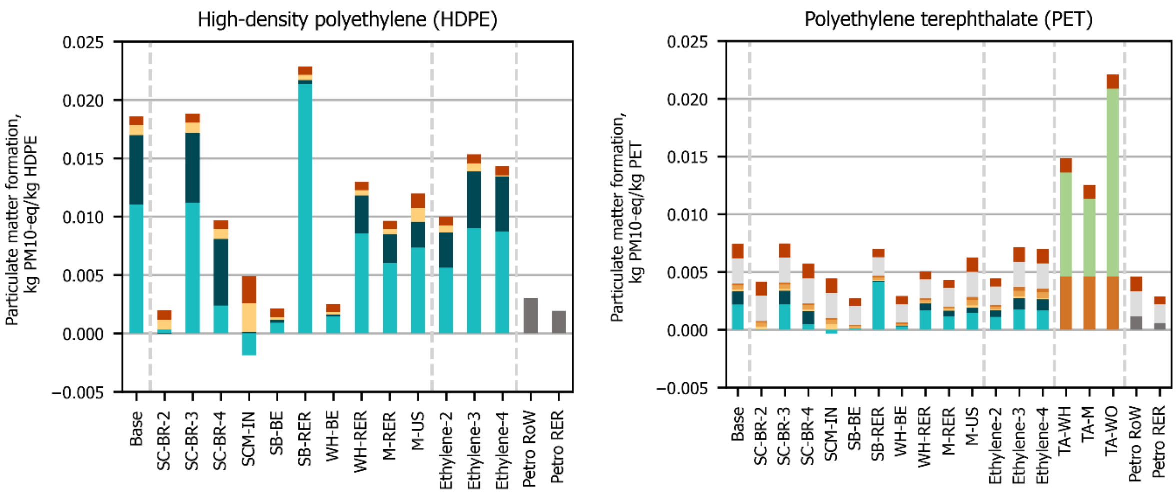


(k) Natural land transformation.

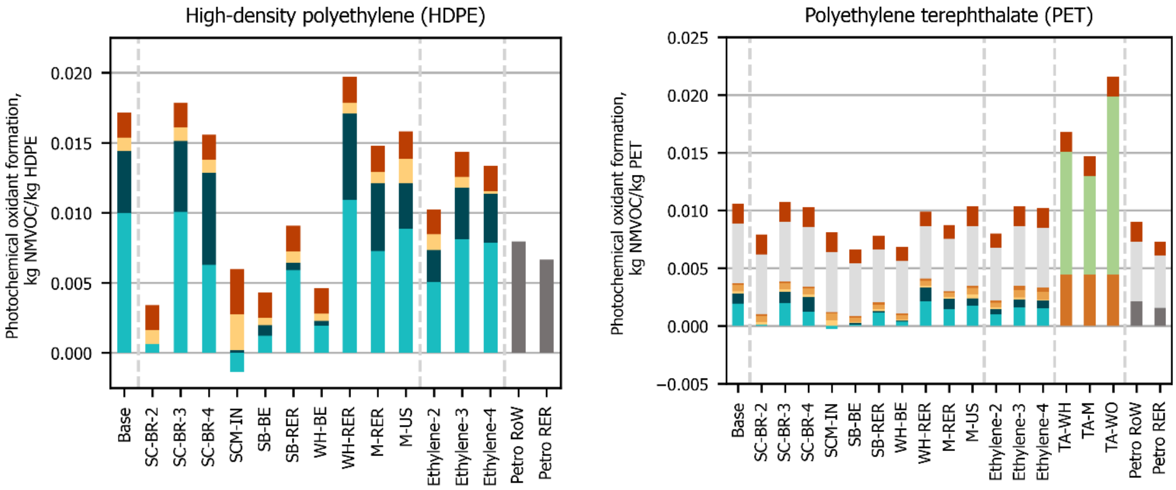


(l) Ozone depletion.

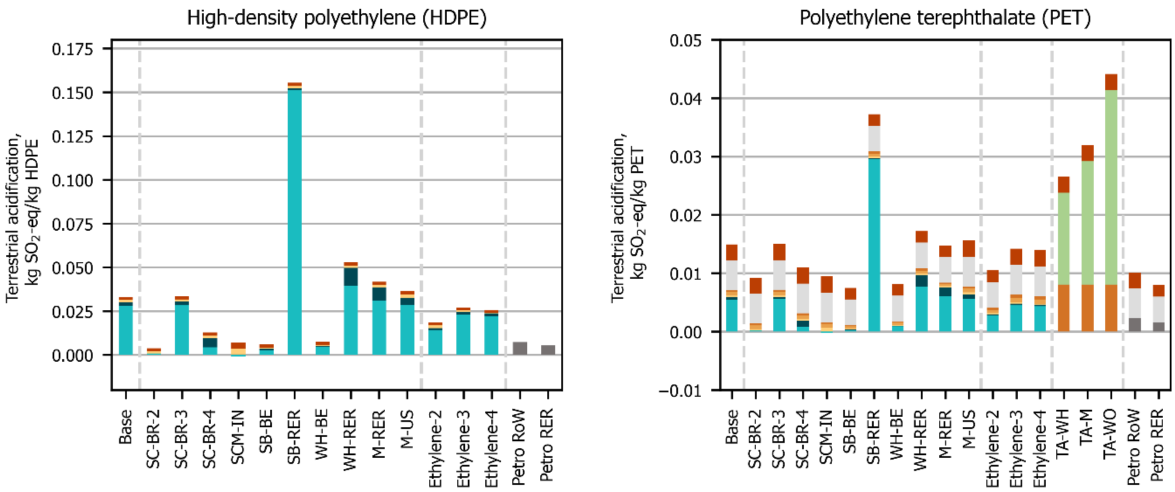
Figure S.2 continued.



(m) Particulate matter formation.

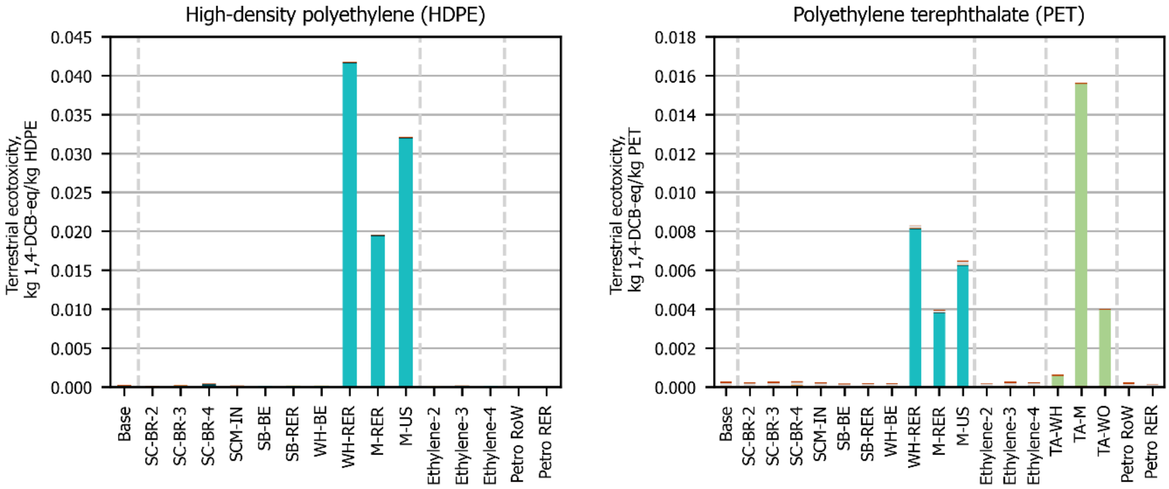


(n) Photochemical oxidant formation.

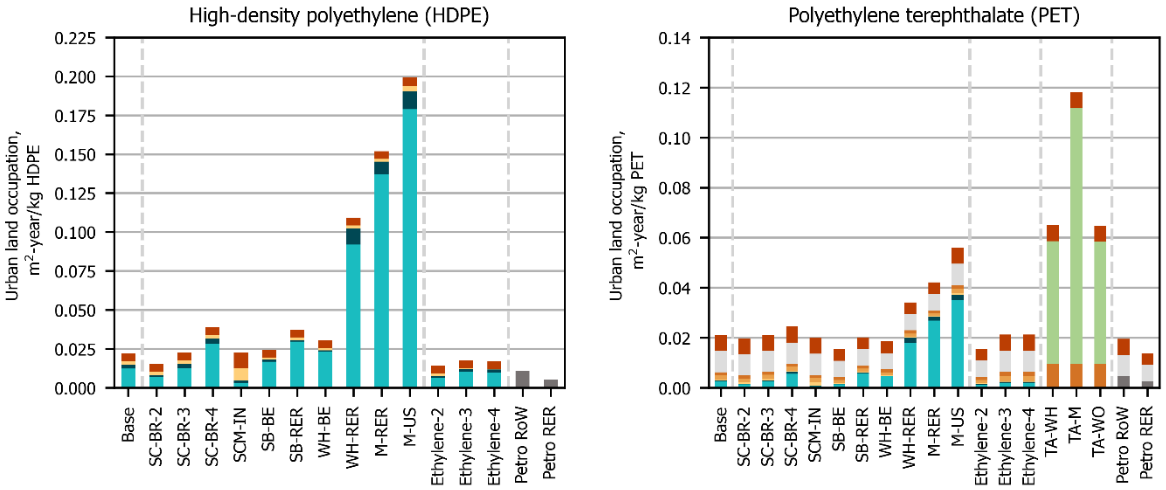


(o) Terrestrial acidification.

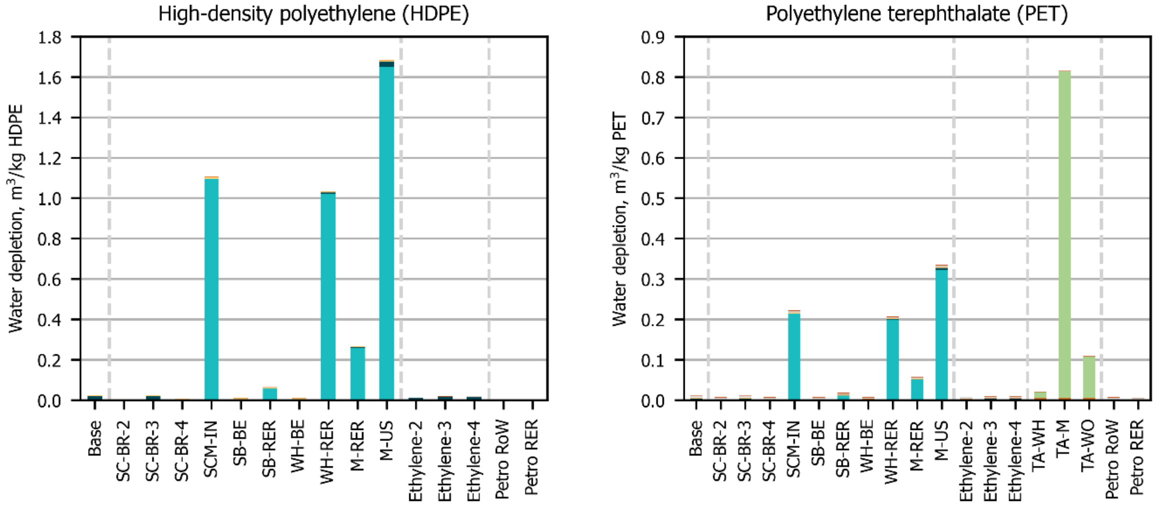
Figure S.2 continued.



(p) Terrestrial ecotoxicity.



(q) Urban land occupation.



(r) Water depletion.

Figure S.2 continued.