Electronic supplementary information 2

Addressing sustainability in photopolymerization: comparative LCA study of six synthetic routes of 1-hydroxycyclohexyl phenyl ketone as photoinitiator for copolymer applications

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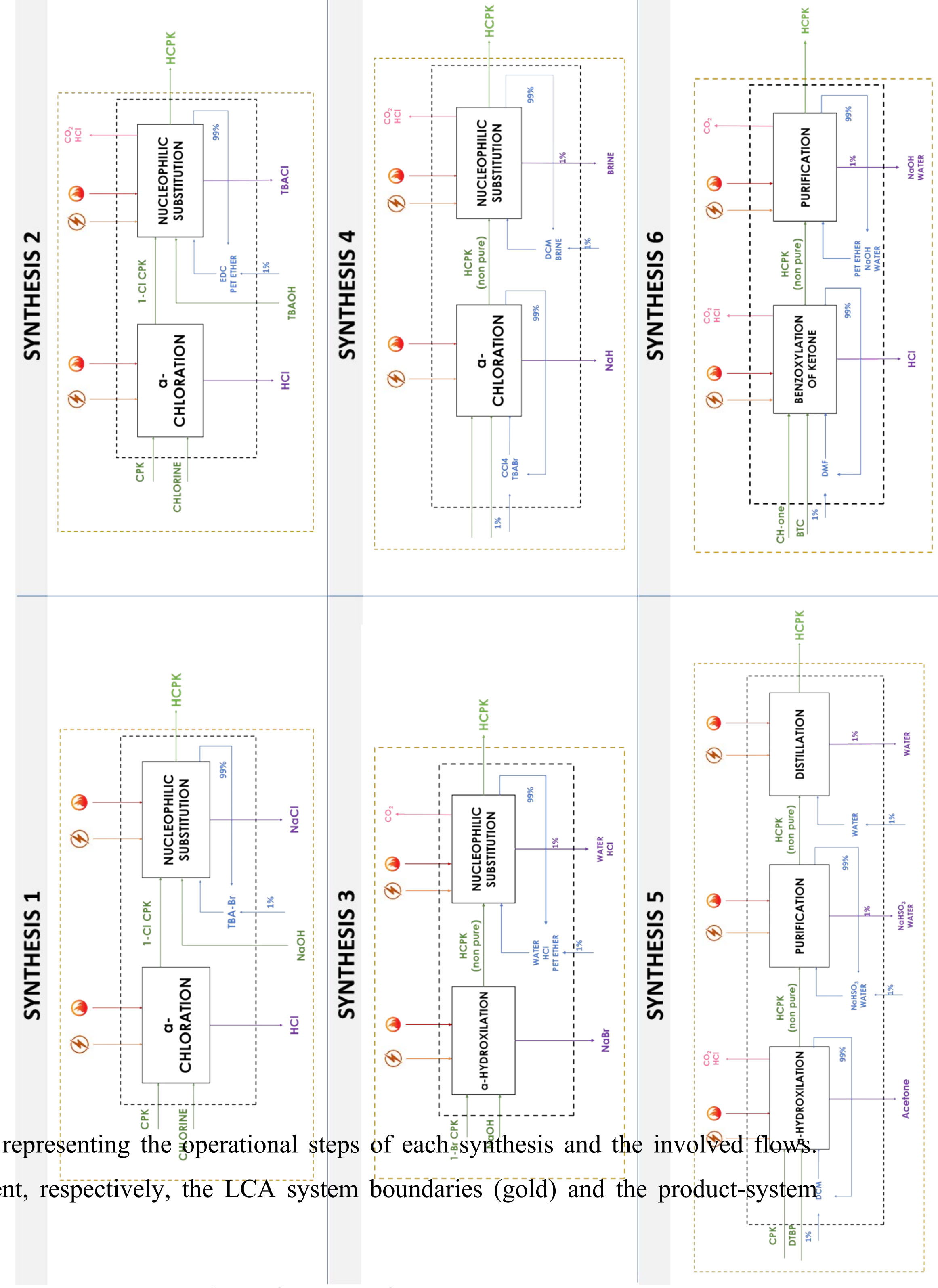


Fig. S1. Flowsheets representing the operational steps of each synthesis and the involved flows. Dashed lines represent, respectively, the LCA system boundaries (gold) and the product-system boundaries (blue).

S1. Description of Irgacure 184 and synthesis pathways

Synthesis 1 (CN111960934A) [1]

Add 15 g of cyclohexyl phenylketone (CPK) to the reactor with the condenser. Chlorine gas (1:2 with respect to the reactant) was introduced for reaction at 70°C for 1.5 h to obtain 17.8 g of compound Cl-CPK. The purity of the liquid phase is 98%, then 15 mL of aqueous solution containing 5 g of sodium hydroxide is added, 0.12 g of tetrabutylammonium bromide (TBA-Br) is reacted at 90°C for about 4.5 h, and then separated. After cooling, 16.05 g of Hydroxy-Cyclohexyl phenyl ketone (HCPK) was obtained as a brown-yellow solid. The yield based on 1-chlorocyclohexyl phenyl ketone is 99%, and the liquid phase purity is 96%.

Synthesis 2 (CN109503343A) [2]

1-Chlorocyclohexyl phenyl ketone (Cl-CPK, 44.5g, 0.2 mol), 100 mL of Dichloroethane is added to the reaction vessel. Stir well and slowly heat to 35°C. A 25% aqueous solution of tetrabutylammonium hydroxide (249.1 g, 0.24 mol) was added dropwise, and the reaction was kept under stirring for 1.5 h. The reaction is carried out under the detection of TLC or GC analysis. After the reaction is completed, the heating and stirring are stopped, the layer is allowed to stand, the organic phase is separated, the aqueous phase is recovered, and the organic phase is washed with water. Then, the hexane was desolvated and recovered, and 80 mL of petroleum ether was added for recrystallisation to obtain a white glossy crystal of 38.0 g (Y=93%), GC content 99.2%.

Synthesis 3 (WO2009135895A1) [3]

6.6 g of 1-Bromocyclohexyl-phenylketone (Br-CPK, 24.7 mmol) were dispersed in 6 g of NaOH 30% and heated to 80 °C; 100 mg of benzyl-triethylammonium chloride were added in two portions, and the mixture was stirred at 80 °C for 1 h. The organic phase was separated and washed warm, with 10 mL of water, then set to pH 3 with concentrated HCl (HCl 37%). The organic phase crystallised from 52.24 g of petroleum ether 40°-65°C, obtaining 3 g of a whitish solid (59%), mp 45°-46°C.

Synthesis 4 (CN108911959A) [4]

In a 1000 ml three-necked flask, 178.7 g of crude CPK, 5.36 g of TBA-Br, 220 g of carbon tetrachloride and 76 g of sodium hydroxide were added, and the condenser was connected. The mixture was heated and stirred at 80-90°C for 12 h. After the reaction was completed, it was cooled to room temperature, diluted with 200 g of dichloromethane, and the organic layer was washed with 180.75 g of saturated brine until neutral. The finished HCPK was 174.8 g, and the yield was 90.2%

Synthesis 5 (CN109694310A) [5]

94.14 g (0.5 mol) of CPK, dichloromethane (DCM) (200 mL), and 231.15 g (5 mol) of di-tert-butyl peroxide (dTBP) were uniformly mixed, placed in an ultrasonic rod (80 kHz), stirred vigorously, and the reaction was controlled. The temperature is around 50°C. The reaction was carried out, and the progress of the reaction was monitored using TLC or GC. After the completion of the reaction, a sodium hydrogen sulfite solution (containing 187.3 g of sodium hydrogen sulfite) was slowly added dropwise to the reaction system to carry out a quenching reaction. Stir until no peroxide is detected with the starch-potassium iodide test paper, then stir for 30 min. Then continue testing with the test paper until there is no peroxide. After standing and layering, the organic layer is washed with 96.00 g of water to neutrality, and 90% of DCM is recovered by atmospheric pressure, and the solvent is further recovered by reducing the pressure. When the solvent and the low-boiling substance were removed, the distillation was carried out under reduced pressure, and a fraction of 107-109°C / 1.8 kPa was collected, and the mixture was cooled to a white solid. 88.47 g of HCPK was obtained, the yield was 86.62%, and the GC content was 99.58%.

Synthesis 6 (CN109896942A) [6]

12 g of 80-100 mesh magnesium powder was dissolved and suspended in 100 mL of DMF (dimethylformamide) solvent, stirred to -20°C (the temperature is reached by using water and NaCl), and 9.8 g of cyclohexanone and 23.46 g of trichloromethylbenzene were dissolved in 40 ml of DMF solvent. Slowly drip into the system of the first step, maintain the system temperature below -20–-10°C for 2 h, naturally warm to room temperature, filter, wash, extract with 34.88 g of petroleum ether, add 30% NaOH 20 g. The aqueous solution and TBA-Br (0.2 g) were controlled to react at a reaction temperature of 50°C for 2 h, and washed with 18.60 g of water and desolvated to obtain 16 g of a product having a purity of 99.6% and a yield of 86%.

S1.1 Inventories of the synthesis

The complete inventories for each examined scenario are reported below. The database records used to model each flow are listed in the last column ("Record"). Records marked with a star (*) were modified or newly developed by the authors. Details on the modelling and modification procedures are provided in Section S1.2. The star marking the electricity records means that the record has been modified according to the Italian electricity mix, as explained in the main text.

Table S1. Inventory of synthesis 1 (S1). All the flows of the three scenarios have been normalized to the functional unit (i.e., 1 kg of HCPK). Electricity consumption of the APC scenario has been estimated in Tables S27 (Step 1) and S28 (Step 2).

				Lab scale	APC	ASPEN	Record
S1	Step 1	Inputs	Cyclohexyl phenylketone (kg)	9.35E-01	9.35E-01	9.22E-01	*Cyclohexyl phenyl ketone (see Table S7)
			Chlorine (kg)	3.01E-01	3.01E-01	3.47E-01	Chlorine, gaseous {RER}| market for chlorine, gaseous | Cut-off, U
			Electricity (kWh)	1.36E+01	5.89E-08	/	*Electricity, medium voltage {IT}| market for | Cut-off, U
			Heat (MJ)	/	3.98E-01	4.43E-02	Heat, central or small-scale, natural gas {RER}| market group for heat, central or small-scale, natural gas | Cut-off, U
		Outputs	1-chlorocyclohexyl phenyl ketone (kg)	1.11E+00	1.00E+03	1.09E+00	/
			HCl (kg)	1.26E-01	1.26E-01	1.78E-01	Spent solvent mixture {Europe without Switzerland}| market for spent solvent mixture | Cut-off, U
	Step 2	Inputs	1-chlorocyclohexyl phenyl ketone (kg)	1.11E+00	1.11E+00	1.09E+00	/
			NaOH (kg)	3.12E-01	3.12E-01	1.96E-01	Sodium hydroxide, without water, in 50% solution state {GLO}| market for sodium hydroxide, without water, in 50% solution state | Cut-off, U
			Tetrabutylammonium bromide (kg)	7.48E-03	7.35E-05	9.57E-05	*Tetrabutylammonium bromide (see Table S12)
			Electricity (kWh)	3.69E+00	2.46E-07	/	*Electricity, medium voltage {IT}| market for | Cut-off, U
			Heat (MJ)	/	5.78E-01	3.75E-01	Heat, central or small-scale, natural gas {RER}| market group for heat, central or small-scale, natural gas | Cut-off, U
		Outputs	1-hydroxycyclohexyl phenyl ketone (kg)	1.00E+00	1.00E+00	1.00E+00	/
			NaCl (kg)	4.28E-01	4.21E-01	2.87E-01	Spent solvent mixture {Europe without Switzerland}| market for spent solvent mixture | Cut-off, U

Table S2. Inventory of synthesis 2 (S2). All the flows of the three scenarios have been normalized to the functional unit (i.e., 1 kg of HCPK). Electricity consumption of the APC scenario has been estimated in Tables S28 (Step 1) and S30 (Step 2).

				Lab scale	APC	ASPEN	Record
S2	Step 1	Inputs	Cyclohexyl phenylketone (kg)	9.87E-01	9.87E-01	9.21E-01	*Cyclohexyl phenyl ketone (see Table S7)
			Chlorine (kg)	3.18E-01	3.18E-01	3.47E-01	Chlorine, gaseous {RER}| market for chlorine, gaseous | Cut-off, U
			Electricity (kWh)	1.44E+01	6.22E-08	/	*Electricity, medium voltage {IT}| market for | Cut-off, U
			Heat (MJ)	/	4.20E-01	4.43E-02	Heat, central or small-scale, natural gas {RER}| market group for heat, central or small-scale, natural gas | Cut-off, U
		Outputs	1-chlorocyclohexyl phenyl ketone (kg)	1.17E+00	1.00E+00	1.09E+00	/
			HCl (kg)	1.34E-01	3.04E-01	1.78E-01	Spent solvent mixture {Europe without Switzerland}| market for spent solvent mixture | Cut-off, U
	Step 2	Inputs	1-chlorocyclohexyl phenyl ketone (kg)	1.17E+00	1.17E+00	1.09E+00	/
			Dichloroethane (kg)	3.29E+00	3.29E-02	2.45E-02	Ethylene dichloride {RER}| market for ethylene dichloride | Cut-off, U
			tetrabutylammonium hydroxide (kg)	1.64E+00	1.64E+00	1.27E+00	*Tetrabutylammonium hydroxide (see Table S20)
			Petroleum ether (kg)	1.37E+00	1.37E-02	1.96E-02	Hexane {GLO}| market for hexane | Cut-off, U
			Heat (MJ)	/	1.07E-01	1.08E+00	Heat, central or small-scale, natural gas {RER}| market group for heat, central or small-scale, natural gas | Cut-off, U
			Electricity (kWh)	8.69E+00	6.67E-08	/	*Electricity, medium voltage {IT}| market for | Cut-off, U
		Outputs	HCPK (kg)	1.00E+00	1.00E+00	1.00E+00	/
			Waste (kg)	1.81E+00	1.81E+00	2.86E-01	Spent solvent mixture {Europe without Switzerland}| market for spent solvent mixture | Cut-off, U
			Carbon dioxide (kg)	7.73E+00	3.63E-02	3.18E-02	Carbon dioxide, into the atmosphere (see Table S22-24)
			HCl (kg)	2.91E+00	2.42E-02	1.80E-02	Hydrochloric Acid, into the atmosphere

Table S3. Inventory of synthesis 3 (S3). All the flows of the three scenarios have been normalized to the functional unit (i.e., 1 kg of HCPK). Electricity consumption of the APC scenario has been estimated in Tables S30 (Step 1) and S31 (Step 2).

				Lab scale	APC	ASPEN	Record
S3	Step 1	Inputs	1-Bromocyclohexyl phenyl ketone (kg)	2.20E+00	2.20E+00	1.31E+00	*1-bromocyclohexyl phenyl ketone (see Table S21)
			Sodium hydroxide (kg)	2.00E+00	2.00E+00	1.96E-01	Sodium hydroxide, without water, in 50% solution state {GLO}| market for sodium hydroxide, without water, in 50% solution state | Cut-off, U
			Cooling energy (kWh)	/	3.32E-01	/	Cooling energy {GLO}| market for cooling energy | Cut-off, U
			Electricity (kWh)	4.84E+00	6.25E-08	/	*Electricity, medium voltage {IT}| market for | Cut-off, U
			Heat (MJ)	/	/	6.61E-01	Heat, central or small-scale, natural gas {RER}| market group for heat, central or small-scale, natural gas | Cut-off, U
		Output	HCPK(non pure) (kg)	1.00E+00	1.00E+00	1.00E+00	/

		s	NaBr (kg)	3.20E+00	3.20E+00	5.04E-01	Spent solvent mixture {Europe without Switzerland}| market for spent solvent mixture | Cut-off, U
	Step 2	Inputs	HCPK (non pure) (kg)	1.00E+00	1.00E+00	1.00E+00	/
			Water (kg)	3.33E+00	3.33E-02	1.98E+00	Water, deionised {Europe without Switzerland}| water production, deionised | Cut-off, U
			HCl (kg)	3.31E-04	3.31E-04	1.96E-04	Hydrochloric acid, without water, in 30% solution state {RER}| market for hydrochloric acid, without water, in 30% solution state | Cut-off, U
			Petroleoum ether (kg)	1.74E+01	1.74E-01	1.04E-01	Hexane {GLO}| market for hexane | Cut-off, U
			Cooling energy (kWh)	/	/	4.52E-02	Cooling energy {GLO}| market for cooling energy | Cut-off, U
			Electricity (kWh)	6.05E+00	4.63E-09	/	*Electricity, medium voltage {IT}| market for | Cut-off, U
		Outputs	HCPK (kg)	1.00E+00	1.00E+00	1.00E+00	/
			Wastewater (kg)	3.33E+00	3.33E-02	5.04E-01	Wastewater, unpolluted {GLO}| market for | Cut-off, U
			Carbon dioxide (kg)	5.35E+01	5.35E-01	3.18E-01	Carbon dioxide, into the atmosphere (see Table S22-24)

Table S4. Inventory of synthesis 4 (S4). All the flows of the three scenarios have been normalized to the functional unit (i.e., 1 kg of HCPK). Electricity consumption of the APC scenario has been estimated in Tables S32 (Step 1) and S33 (Step 2). The production of saturated brine is simulated by using 0.26 kg of sodium chloride (Sodium chloride, powder {GLO}| market for sodium chloride, powder | Cut-off, U) and 0.74 kg of water (Water, deionised {Europe without Switzerland}| market for water, deionised | Cut-off, U)

				Lab scale	APC	ASPEN	Record
S4	Step 1	Inputs	Cyclohexyl phenylketone (kg)	9.22E-01	9.22E-01	8.94E-01	*Cyclohexyl phenyl ketone (see Table S7)
			Tetrabutylammonium bromide (kg)	2.77E-02	2.77E-04	2.68E-04	*Tetrabutylammonium bromide (see Table S12)
			Carbon tetrachloride (kg)	1.14E+00	1.14E-02	2.97E-01	Carbon tetrachloride {RER}| market for carbon tetrachloride | Cut-off, U
			Sodium hydroxide (kg)	3.92E-01	3.92E-01	3.09E-01	Sodium hydroxide, without water, in 50% solution state {GLO}| market for sodium hydroxide, without water, in 50% solution state | Cut-off, U
			Electricity (kWh)	7.08E+00	7.25E-07	/	*Electricity, medium voltage {IT}| market for | Cut-off, U
			Heat (MJ)	/	4.37E+00	1.95E+00	Heat, central or small-scale, natural gas {RER}| market group for heat, central or small-scale, natural gas | Cut-off, U
		Outputs	1-chlorocyclohexyl phenyl ketone (kg)	1.00E+00	1.00E+00	1.00E+00	/
			Waste (kg)	1.48E+00	3.26E-01	2.68E-04	Spent solvent mixture {Europe without Switzerland}| market for spent solvent mixture | Cut-off, U
	Step 2	Inputs	HCPK (non pure) (kg)	1.00E+00	1.00E+00	1.00E+00	/
			Saturated brine (kg)	9.33E-01	9.33E-03	9.04E-03	*Saturated brine (see Table caption)
			Dichloromethane (kg)	1.00E+00	1.03E-02	1.00E-02	Dichloromethane {RER}| market for dichloromethane | Cut-off, U

			Cooling energy (kWh)	/	/	5.81E-02	Cooling energy {GLO}| market for cooling energy | Cut-off, U
			Electricity (kWh)	/	5.14E-07	3.64E-05	*Electricity, medium voltage {IT}| market for | Cut-off, U
		Outputs	HCPK (kg)	1.00E+00	1.00E+00	1.00E+00	/
			Waste (kg)	9.33E-01	9.33E-03	6.86E-01	Spent solvent mixture {Europe without Switzerland}| market for spent solvent mixture | Cut-off, U
			Carbon dioxide (kg)	5.18E-01	5.35E-03	5.18E-03	Carbon dioxide, into the atmosphere (see Table S22-24)
			HCl (kg)	8.59E-01	8.86E-03	8.59E-03	Hydrochloric Acid, into the atmosphere (see Table S22-24)

Table S5. Inventory of synthesis 5 (S5). All the flows of the three scenarios have been normalized to the functional unit (i.e., 1 kg of HCPK). Electricity consumption of the APC scenario has been estimated in Tables S34 (Step 1) and S35 (Step 2). The production of di-butyl-peroxide has been simulated according to Minkoff et al. (1954) [7]

				Lab scale	APC	ASPEN	Record
S5	Step 1	Inputs	Cyclohexyl phenylketone (kg)	1.06E+00	1.06E+00	5.12E-01	*Cyclohexyl phenyl ketone (see Table S7)
			Di-tert-butyl peroxide (kg)	2.61E+00	2.61E+00	2.62E+00	*Di-tert-butyl peroxide (see Table caption)
			Dichloromethane (kg)	3.01E-01	3.01E-03	3.02E-01	Dichloromethane {RER}| market for dichloromethane | Cut-off, U
			Cooling energy (kWh)	/	/	5.70E-02	Cooling energy {GLO}| market for cooling energy | Cut-off, U
			Electricity (kWh)	5.95E+00	4.63E-06	/	*Electricity, medium voltage {IT}| market for | Cut-off, U
			Heat (MJ)	/	7.13E-02	/	Heat, central or small-scale, natural gas {RER}| market group for heat, central or small-scale, natural gas | Cut-off, U
		Outputs	HCPK (non pure) (kg)	1.04E+00	1.04E+03	9.95E+02	/
			Waste (kg)	2.64E+00	2.64E+00	2.14E+00	Spent solvent mixture {Europe without Switzerland}| market for spent solvent mixture | Cut-off, U
			Carbon dioxide (kg)	1.56E-01	1.56E-03	1.56E-01	Carbon dioxide, into the atmosphere (see Table S22-24)
			HCl (kg)	2.58E-01	2.58E+00	2.58E+02	Hydrochloric Acid, into the atmosphere (see Table S22-24)
	Step 2	Inputs	HCPK (non pure) (kg)	1.04E+00	1.04E+00	1.00E+00	/
			Sodium hydrogen sulfite (kg)	2.04E+00	2.12E-02	2.13E-02	Sodium hydrogen sulfite {GLO}| market for sodium hydrogen sulfite | Cut-off, U
			Water (kg)	2.19E+00	4.92E-05	4.97E-05	Water, deionised {Europe without Switzerland}| water production, deionised | Cut-off, U
			Cooling energy (kWh)	/	/	2.64E-01	Cooling energy {GLO}| market for cooling energy | Cut-off, U
			Electricity (kWh)	8.51E-01	3.72E-08	/	*Electricity, medium voltage {IT}| market for | Cut-off, U
		Outputs	HCPK (kg)	1.04E+00	1.04E+00	1.00E+00	/
			Wastewater (kg)	2.19E+00	4.92E-05	4.97E-05	Wastewater, unpolluted {GLO}| market for | Cut-off, U
			Waste (kg)	2.04E+00	2.12E-02	2.13E-02	Spent solvent mixture {Europe without Switzerland}| market for spent solvent mixture | Cut-off, U
	Step 3	Inputs	HCPK (non pure) (kg)	1.04E+00	1.04E+00	1.00E+00	/
			Water (kg)	1.09E+00	1.09E-02	1.09E-02	Water, deionised {Europe without Switzerland}| water production, deionised | Cut-off, U
			Cooling energy (kWh)	/	/	3.44E-03	Cooling energy {GLO}| market for cooling energy | Cut-off, U
			Electricity (kWh)	8.09E-01	/	/	*Electricity, medium voltage {IT}| market for | Cut-off, U
			Heat (MJ)	/	8.23E-01	7.07E-02	Heat, central or small-scale, natural gas {RER}| market group for heat, central or small-scale, natural gas | Cut-off, U

				Lab scale	APC	ASPEN	Record
		Outputs	HCPK (kg)	1.00E+00	1.00E+00	1.00E+00	/
			Waste (kg)	1.13E+00	1.09E-02	1.09E-02	Spent solvent mixture {Europe without Switzerland}| market for spent solvent mixture | Cut-off, U

Table S6. Inventory of synthesis 6 (S6). All the flows of the three scenarios have been normalized to the functional unit (i.e., 1 kg of HCPK). Electricity consumption of the APC scenario has been estimated in Tables S36 (Step 1) and S37 (Step 2). The production of benzotrichloride is simulated according to the patent JP5647782 [8]. It has been modelled by mixing 0.471 kg of toluene (Toluene, liquid {RER}| market for toluene, liquid | Cut-off, U) and 1.088 kg of chlorine. Since the reaction occurs at 20°C, the heat consumption has been neglected.

				Lab scale	APC	ASPEN	Record
S6	Step 1	Inputs	Benzothrichloride (kg)	1.47E+00	1.47E+00	4.23E-01	*Benzotrichloride (see Table caption)
			N,N dimethyl formamide (kg)	1.06E+01	8.75E-02	1.37E-01	N,N-dimethylformamide {GLO}| market for N,N-dimethylformamide | Cut-off, U
			Cyclohexanone (kg)	6.13E-01	6.12E-01	9.61E-01	Cyclohexanone {RER}| market for cyclohexanone | Cut-off, U
			Electricity (kWh)	1.82E+01	7.95E-08	/	*Electricity, medium voltage {IT}| market for | Cut-off, U
		Outputs	HCPK (non pure) (kg)	1.16E+00	1.16E+00	1.00E+00	/
			Carbon dioxide (kg)	2.62E+00	1.84E-01	2.48E-01	Carbon dioxide, into the atmosphere (see Table S22-24)
			Nitrogen dioxide (kg)	9.14E-01	6.40E-02	8.64E-02	Nitrogen dioxide, into the atmosphere (see Table S22-24)
	Step 2	Inputs	HCPK (non pure) (kg)	1.16E+00	1.16E+00	1.00E+00	/
			Petroleoum ether (kg)	1.45E+00	2.18E-02	3.98E-02	Hexane {GLO}| market for hexane | Cut-off, U
			Sodium hydroxide (kg)	1.25E+00	3.75E-01	6.84E-01	Sodium hydroxide, without water, in 50% solution state {GLO}| market for sodium hydroxide, without water, in 50% solution state | Cut-off, U
			Water (kg)	1.16E+00	1.16E-02	2.12E-02	Water, deionised {Europe without Switzerland}| water production, deionised | Cut-off, U
			Cooling energy (kWh)	/	1.55E+01	9.00E+00	Cooling energy {GLO}| market for cooling energy | Cut-off, U
			Electricity (kWh)	8.46E-01	/	3.92E-06	*Electricity, medium voltage {IT}| market for | Cut-off, U
		Outputs	HCPK (kg)	1.00E+00	1.00E+00	1.00E+00	/
			Carbon dioxide (kg)	4.46E+00	6.69E-02	1.22E-01	Carbon dioxide, into the atmosphere (see Table S22-24)
			Wastewater (kg)	2.58E+00	1.16E-02	2.12E-02	Wastewater, unpolluted {GLO}| market for | Cut-off, U
			Waste (kg)	1.25E+00	3.75E-01	6.84E-01	Spent solvent mixture {Europe without Switzerland}| market for spent solvent mixture | Cut-off, U

S1.2 Modelling of reagents not available in the database

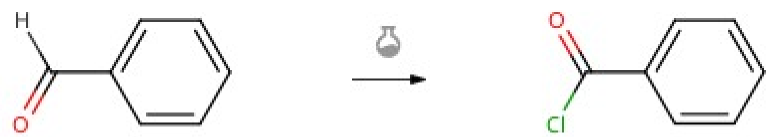
The models include the amount of reagent employed in the reaction and the energy consumption to heat or cool the reaction. The use of catalysts and auxiliaries, which can potentially be recovered, is always neglected. All the models have been generated according to the information reported in Reaxys [9].

- ***Cyclohexylphenylketone***

The synthesis consists of three steps. In the first step, benzaldehyde and Cl_2, in the presence of chlorine, react to produce benzoyl chloride and hydrochloric acid (Figure S2).

Table S7. Inventory used for the modelling of Benzoyl chloride production

Reaction ID: 601767	n°mol	MM	m (1kg)	Record
Benzaldeyde	1	106.12	7.55E-01	Benzaldehyde {GLO}| market for | Cut-off, U
Cl_2	1	70.91	5.04E-01	Chlorine, liquid {GLO}| market for | Cut-off, U
Benzoyl chloride	1	140.57	1.00E+00	_Benzoyl chloride (GLO)
HCl	1	36.46	2.59E-01	Spent solvent mixture {Europe without Switzerland}| market for spent solvent mixture | Cut-off, U



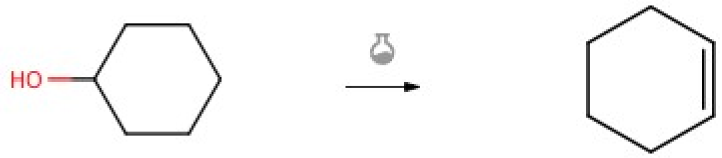
$$C_7H_6O + Cl_2 \rightarrow C_7H_5ClO + HCl$$

Fig. S2. Synthesis of benzoyl chloride according to reaction ID 601767

In a parallel step, cyclohexanol is converted into cyclohexene, adding sulfuric acid at 250°C for 30 minutes.

Table S8. Inventory used for the modelling of Cyclohexene

Reaction ID: 824879	n°mol	MM	m (1kg)	Record
Cyclohexanol	1	100.16	1.22E+00	Cyclohexanol {GLO}| market for | Cut-off, U
Cyclohexene	1	82.15	1.00E+00	_Cyclohexene
H_2O	1	18.02	2.19E-01	Wastewater, unpolluted {GLO}| market for | Cut-off, U



$C_6H_{12}O_6 \rightarrow C_6H_{10} + H_2O$

Fig. S3. Synthesis of benzoyl chloride according to reaction ID 824879

The estimated heat consumption is 0.19 MJ/kg of product.

Table S9. Heating energy estimated for the production of Cyclohexene.

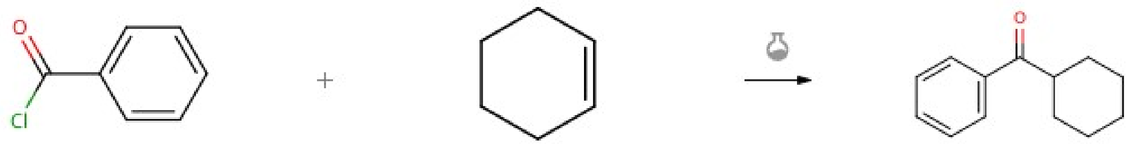
Inputs	Mass (kg)	Mass (%)
Cyclohexanol	1.22	100.0%
Heat	2.52E+03	MJ

Q_{react}	2.52E+03	MJ
η_{HEAT}	7.50E-01	/
Q_{heat}	5.23E+02	MJ
C_p	2.28E+03	J/kg*K
m_{mix}	1.00E+03	kg
T_r	5.23E+02	K
T_0	2.93E+02	K
Q_{loss}	1.37E+03	MJ
Q_{loss}	1.37E+09	W/s (=J)
A	5.90E+03	m^2
k_a/s	5.60E-01	W/(m^2*k)
T_r	5.23E+02	K
T_{out}	2.93E+02	K
time	1.80E+03	s

Finally, cyclohexene, benzoyl chloride and cyclohexane react to give CPK and chloro-cyclohexane. An ambient of aluminium chloride at -10-60°C is required to perform the reaction.

Table S10. Inventory used for the modelling of CPK

Reaction ID: 615820	n°mol	MM	m (1kg)	Record
Benzoyl chloride	1	140.57	7.47E-01	_Benzoyl chloride (GLO)
Cyclohexene	1	82.15	4.36E-01	_Cyclohexene
Cyclohexane	1	84.16	4.47E-01	Cyclohexane {GLO}| market for cyclohexane | Cut-off, U
CPK	1	188.27	1.00E+00	_Cyclohexyl phenyl ketone
Cl-Cyclohexane	1	118.60	6.30E-01	Spent solvent mixture {Europe without Switzerland}| market for spent solvent mixture | Cut-off, U



$C_7H_5ClO + C_6H_{10} + C_6H_{12} \rightarrow C_6H_{12}COC_6H_5 + C_6H_{11}Cl$

Fig. S4. Synthesis of CPK according to reaction ID 615820

Table S11. Heating energy estimated for the production of CPK.

Inputs	Mass (kg)	Mass (%)
Benzoyl chloride	7.47E-01	63.1%
Cyclohexene	4.36E-01	36.9%
Heat	1.94E+02	MJ

$Cp_{benzoyl\ chloride}$	1.44E+03
$Cp_{cyclohexene}$	2.04E+03
Weighted average	1.66E+03

$\mathbf{Q_{react}}$	1.94E+02	MJ
η_{HEAT}	7.50E-01	/
Q_{heat}	6.64E+01	MJ
C_p	1.66E+03	J/kg*K
m_{mix}	1.00E+03	kg
T_r	3.33E+02	K
T_0	2.93E+02	K
Q_{loss}	7.93E+01	MJ
Q_{loss}	7.93E+07	W/s (=J)
A	5.90E+03	m^2
k_a/s	5.60E-01	$W/(m^2*k)$
T_r	3.33E+02	K
T_{out}	2.93E+02	K
time	6.00E+02	s

- ***Tertbutylammonium bromide***

The synthesis consists of four steps. In the first step, Br_2 and water are irradiated to give hydrogen bromide and HOBr. The Reaxys reaction ID is 26086676.

Table S12. Inventory used for the modelling of Hydrogen bromide

Reaction ID: 26086676	n°mol	MM	m (1kg)	Record
Br_2	1	159.81	1.98E+00	Bromine {GLO}| market for bromine | Cut-off, U
Water	1	18.02	2.23E-01	Water, ultrapure {RER}| market for water, ultrapure | Cut-off, U
Hydrogen bromide	1	80.91	1.00E+00	_hydrogen bromide
HOBr	1	96.91	1.20E+00	Spent solvent mixture {Europe without Switzerland}| market for spent solvent mixture | Cut-off, U

The estimated heat consumption is 22.9 MJ/kg of product.

Table S13. Heating energy estimated for the production of HBr.

Inputs	Mass (kg)	Mass (%)
Br_2	1.975133	89.9%
Water	0.222655	10.1%
Heat	2.29E+04	MJ

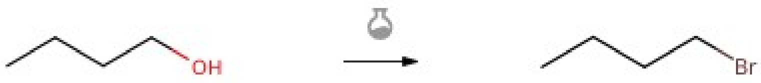
C_p	J/kg*K
Cp_{Br2}	2.29E+02
Cp_{Water}	4.20E+03
Weighted average	6.31E+02

Q_{react}	2.29E+04	MJ
η_{HEAT}	7.50E-01	/
Q_{heat}	3.78E+01	MJ
C_p	6.31E+02	J/kg*K
m_{mix}	1.00E+03	kg
T_r	3.53E+02	K
T_0	2.93E+02	K
Q_{loss}	1.71E+04	MJ
Q_{loss}	1.71E+10	W/s (=J)
A	5.90E+03	m^2
k_a/s	5.60E-01	W/(m^2*k)
T_r	3.53E+02	K
T_{out}	2.93E+02	K
time	8.64E+04	s

The second step consists of the reaction of hydrogen bromide with butanol to obtain bromobutane. The reaction is performed in water at 80°C for 24h.

Table S14. Inventory used for the modelling of Bromobutane.

Reaction ID: 845422	n°mol	MM	m (1kg)	Record
Butanol	1	74.12	5.41E-01	N-butanol {GLO}| market for n-butanol | Cut-off, U
HBr	1	80.91	5.91E-01	_hydrogen bromide
Br-butane	1	137.02	1.00E+00	_1-bromo-butane
H_2O	1	18.02	1.31E-01	Wastewater, unpolluted {GLO}| market for | Cut-off, U



$$C_4H_9OH + HBr \rightarrow C_4H_9Br + H_2O$$

Fig. S5. Synthesis of Bromo-butane according to reaction ID 845422.

The estimated heat consumption is 23.0 MJ/kg of product.

Table S15. Heating energy estimated for the production of Bromobutane.

Inputs	Mass (kg)	Mass (%)
Butanol	5.41E-01	47.8%
HBr	5.91E-01	52.2%
Heat	2.30E+04	MJ

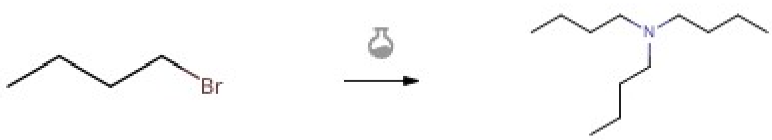
C_p	J/kg*K
$Cp_{butanol}$	2.61E+03
Cp_{HBr}	4.11E+02
Weighted average	1.46E+03

Q_{react}	2.30E+04	MJ
η_{HEAT}	7.50E-01	/
Q_{heat}	8.77E+01	MJ
C_p	1.46E+03	J/kg*K
m_{mix}	1.00E+03	kg
T_r	3.53E+02	K
T_0	2.93E+02	K
Q_{loss}	1.71E+04	MJ
Q_{loss}	1.71E+10	W/s (=J)
A	5.90E+03	m^2
k_a/s	5.60E-01	W/(m^2*k)
T_r	3.53E+02	K
T_{out}	2.93E+02	K
time	8.64E+04	s

The third step consists of the reaction of bromobutane with urea to obtain tributylamine and ammonium bromide, and carbon dioxide. The reaction occurs in an ambient of sodium hydroxide, at 120°C, under 3103 Torr, for 40 h.

Table S16. Inventory used for the modelling of tributylamine.

Reaction ID: 58918	n°mol	MM	m (1kg)	Record
Br-butane	3	137.02	2.22E+00	_1-bromo-butane
Urea	1	60.06	3.24E-01	Urea {RER}| market for urea | Cut-off, U
Tributylamine	1	185.35	1.00E+00	_tributyl-amine
Ammonium bromide	2	97.94	1.06E+00	Spent solvent mixture {Europe without Switzerland}| market for spent solvent mixture | Cut-off, U
CO_2	1	44.01	2.37E-01	/



$$C_4H_9Br + CH_4N_2O \rightarrow C_{12}H_{27}N + NH_4Br + CO_2$$

Fig. S6. Synthesis of tributylamine according to reaction ID 58918.

The estimated heat consumption is 63.7 MJ/kg of product.

Table S17. Heating energy estimated for the production of tributylamine.

Inputs	Mass (kg)	Mass (%)
Br-butane	2.217698	87.3%
Urea	0.32403	12.7%
Heat	6.37E+04	MJ

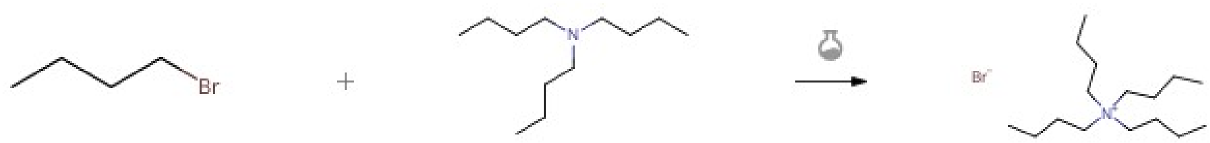
C_p	J/kg*K
$Cp_{butanol}$	2.61E+03
Cp_{HBr}	4.12E+02
Weighted average	2.33E+03

Q_{react}	6.37E+04	MJ
η_{HEAT}	7.50E-01	/
Q_{heat}	2.33E+02	MJ
C_p	2.33E+03	J/kg*K
m_{mix}	1.00E+03	kg
T_r	3.93E+02	K
T_0	2.93E+02	K
Q_{loss}	4.76E+04	MJ
Q_{loss}	4.76E+10	W/s (=J)
A	5.90E+03	m^2
k_a/s	5.60E-01	$W/(m^2*k)$
T_r	3.93E+02	K
T_{out}	2.93E+02	K
time	1.44E+05	s

The fourth step consists of the reaction of tributylamine and bromobutane, in acetonitrile, at 82°C, for 33 h, to obtain TBA-Br.

Table S18. Inventory used for the modelling of TBA-Br.

Reaction ID: 58677	n°mol	MM	m (1kg)	Record
Br-butane	1	185.35	5.75E-01	_1-bromo-butane
Tributylamine	1	137.02	4.25E-01	_tributyl-amine
TBA-Br	1	322.37	1.00E+00	_tetrabutylammonium bromide



$$C_4H_9Br + C_{12}H_{27}N \rightarrow C_{16}H_{36}BrN$$

Fig. S7. Synthesis of tributylamine according to reaction ID 58677 XY

The estimated heat consumption is 32.6 MJ/kg of product.

Table S19. Heating energy estimated for the production of trimethylamine.

Inputs	Mass (kg)	Mass (%)
Br-butane	5.75E-01	57.5%
Tributylamine	4.25E-01	42.5%
Heat	3.26E+04	MJ

C_p	J/kg*K
$Cp_{Br\text{-}butane}$	1.25E+03
$Cp_{Tributylammine}$	2.33E+03
Weighted average	1.71E+03

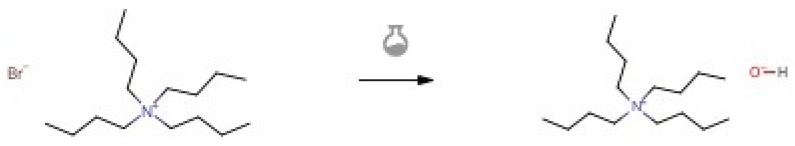
Q_{react}	3.26E+04	MJ
η_{HEAT}	7.50E-01	/
Q_{heat}	1.06E+02	MJ
C_p	1.71E+03	J/kg*K
m_{mix}	1.00E+03	kg
T_r	3.55E+02	K
T_0	2.93E+02	K
Q_{loss}	2.43E+04	MJ
Q_{loss}	2.43E+10	W/s (=J)
A	5.90E+03	m^2
k_a/s	5.60E-01	$W/(m^2*k)$
T_r	3.55E+02	K
T_{out}	2.93E+02	K
time	1.19E+05	s

- ***Tertbutylammoniumhydroxide***

The production of tetrabutylammonium hydroxide (TBA-OH) consists of the reaction between TBA-Br and potassium hydroxide, at 20°C, in dichloromethane, for 10h.

Table S20. Inventory used for the modelling of TBA-OH.

Reaction ID: 2238232	n°mol	MM	m (1kg)	Record
TBA-Br	1	322.37	1.24E+00	_tetrabutylammonium bromide
KOH	1	56.11	2.16E-01	Potassium hydroxide {GLO}| market for potassium hydroxide | Cut-off, U
TBA-OH	1	259.48	1.00E+00	_tetrabutylammonium hydroxide
KBr	1	119.00	4.59E-01	Spent solvent mixture {Europe without Switzerland}| market for spent solvent mixture | Cut-off, U



$$C_{16}H_{36}BrN \rightarrow C_{16}H_{36}OHN$$

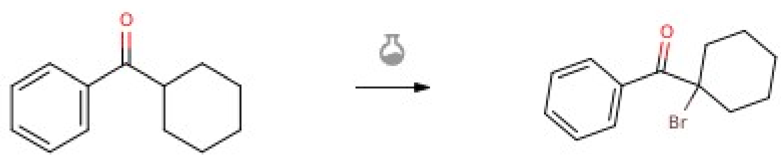
Fig. S8. Synthesis of TBA-OH according to reaction ID 2238232 [9]

- ***Cyclohexylphenylketonebromide***

The production of Br-CPK consists of the reaction between CPK and HBr, in the presence of dimethyl sulfoxide, water, ethyl acetate, at 60°C, for 6h.

Table S21. Inventory used for the modelling of Br-CPK.

Reaction ID: 615820	n°mol	MM	m (1kg)	Record
CPK	1	188.27	7.05E-01	_Cyclohexyl phenyl ketone
HBr	1	80.91	3.03E-01	_hydrogen bromide
Br-CPK	1	267.17	1.00E+00	_1-bromocyclohexyl phenyl ketone



$$C_6H_{12}COC_6H_5 \rightarrow C_6H_{11}BrCOC_6H_5$$

Fig. S9. Synthesis of TBA-OH according to reaction ID 615820

The estimated heat consumption is 3.88 MJ/kg of product.

Inputs	Mass (kg)	Mass (%)
Cyclohexyl phenyl ketone	0.704689	69.9%
HBr	0.302845	30.1%
Heat	3.88E+03	MJ

C_p	J/kg*K
Cp_{CPK}	1.78E+03
Cp_{HBr}	4.11E+02
Weighted average	1.37E+03

Q_{react}	3.88E+03	MJ
η_{HEAT}	7.50E-01	/
Q_{heat}	5.47E+01	MJ
C_p	1.37E+03	J/kg*K
m_{mix}	1.00E+03	kg
T_r	3.33E+02	K
T_0	2.93E+02	K
Q_{loss}	2.85E+03	MJ
Q_{loss}	2.85E+09	W/s (=J)
A	5.90E+03	m^2
k_a/s	5.60E-01	$W/(m^2*k)$
T_r	3.33E+02	K
T_{out}	2.93E+02	K
time	2.16E+04	s

S2. Emission profiles

The emission profiles associated with the combustion of substances released into the environment are reported in Tables S22–S24. The amounts of CO_2 and other oxidation products were calculated on a stoichiometric basis. The emitted quantities were subsequently calculated proportionally. Tables S22–S24 list the compounds subject to oxidation in the different processes investigated (i.e., dichloroethane, hexane, dichloromethane, and N,N-dimethylformamide). Since some substances were common to multiple syntheses, the cells highlighted in yellow report the quantities emitted for each substance according to the specific syntheses indicated in the first column (e.g., Synthesis 2, Synthesis 3, etc.).

Table S22. Emission profiles according to stoichiometry (Lab Scale)

	Dichloroethane	**$C_2H_4Cl_2$**	**O_2**		**CO_2**	**H_2O**	**HCl**
	n mol	1	2.5		2	1	2
	MM (g/mol)	9.90E+01	3.20E+01	→	4.40E+01	1.80E+01	3.65E+01
	m (g)	9.90E+01	8.00E+01		8.80E+01	1.80E+01	7.29E+01
synthesis 2a	**m lab (g)**	*1.50E+02*			*1.33E+02*		*1.10E+02*
	Hexane	**C_6H_{14}**	**O_2**		**CO_2**	**H2O**	
	n mol	1	9.5		6	7	
	MM (g/mol)	8.60E+01	3.20E+01		4.40E+01	1.80E+01	
	m (g)	8.60E+01	3.04E+02	→	2.64E+02	1.26E+02	
synthesis 2a	**m lab (g)**	*5.22E+01*			*1.60E+02*		
synthesis 3	**m lab (g)**	*5.22E+01*			*1.60E+02*		
synthesis 6	**m scale-up (g)**	*2.32E+01*			*7.13E+01*		
	Dichloromethane	**CCl_2H_2**	**O_2**		**CO_2**	**HCl**	
	n mol	1	1		1	2	
	MM (g/mol)	8.49E+01	3.20E+01	→	4.40E+01	3.65E+01	
	m (g)	8.49E+01	3.20E+01		4.40E+01	7.29E+01	
synthesis 4	**m lab (g)**	*1.94E+02*			*1.00E+02*	*1.66E+02*	
synthesis 5	**m lab (g)**	*2.66E+01*			*1.38E+01*	*2.28E+01*	
	N,N dimethyl formamide	**C_3H_7NO**	**O_2**		**CO_2**	**H_2O**	**NO_2**
	n mol	2	10.5		6	7	2
	MM (g/mol)	7.31E+01	3.20E+01	→	4.40E+01	1.80E+01	4.60E+01
	m (g)	1.46E+02	3.36E+02		2.64E+02	1.26E+02	9.20E+01
synthesis 6.1	**m lab (g)**	*2.32E+01*			*4.20E+01*		*1.46E+01*

Table S23. Emission profiles according to stoichiometry (APC)

	Dichloroethane	**$C_2H_4Cl_2$**	**O_2**		**CO_2**	**H2O**	**HCl**
	n mol	1	2.5	→	2	1	2
	MM (g/mol)	9.90E+01	3.20E+01		4.40E+01	1.80E+01	3.65E+01
	m (g)	9.90E+01	8.00E+01		8.80E+01	1.80E+01	7.29E+01
synthesis 2a	**m scale-up (g)**	*3.29E+01*			*2.93E+01*		*2.42E+01*
	Hexane	**C_6H_{14}**	**O_2**		**CO_2**	**H2O**	
	n mol	1	9.5		6	7	
	MM (g/mol)	8.60E+01	3.20E+01		4.40E+01	1.80E+01	
	m (g)	8.60E+01	3.04E+02	→	2.64E+02	1.26E+02	
synthesis 2a	**m scale-up (g)**	*1.37E+01*			*7.03E+00*		
synthesis 3	**m scale-up (g)**	*1.74E+02*			*5.35E+02*		
synthesis 6	**m scale-up (g)**	*2.18E+01*			*6.69E+01*		
	Dichloromethane	**CCl_2H_2**	**O_2**		**CO_2**	**HCl**	
	n mol	1	1		1	2	
	MM (g/mol)	8.49E+01	3.20E+01	→	4.40E+01	3.65E+01	
	m (g)	8.49E+01	3.20E+01		4.40E+01	7.29E+01	
synthesis 4	**m scale-up (g)**	*1.03E+01*			*5.35E+00*	*8.86E+00*	
synthesis 5	**m scale-up (g)**	*3.01E+00*			*1.56E+00*	*2.58E+00*	
	N,N dimethyl formamide	**C_3H_7NO**	**O_2**		**CO_2**	**H_2O**	**NO_2**
	n mol	2	10.5		6	7	2
	MM (g/mol)	7.31E+01	3.20E+01	→	4.40E+01	1.80E+01	4.60E+01
	m (g)	1.46E+02	3.36E+02		2.64E+02	1.26E+02	9.20E+01
synthesis 6.1	**m scale-up (g)**	*8.75E+01*			*1.58E+02*		*5.51E+01*

Table S24. Emission profiles according to stoichiometry (SAM)

	Dichloroethane	**$C_2H_4Cl_2$**	**O_2**		**CO_2**	**H_2O**	**HCl**
	n mol	1	2.5		2	1	2
	MM (g/mol)	9.90E+01	3.20E+01	→	4.40E+01	1.80E+01	3.65E+01
	m (g)	9.90E+01	8.00E+01		8.80E+01	1.80E+01	7.29E+01
synthesis 2a	**m scale-up (g)**	*2.63E+01*			*2.34E+01*		*1.94E+01*
	Hexane	**C_6H_{14}**	**O_2**		**CO_2**	**H_2O**	
	n mol	1	9.5		6	7	
	MM (g/mol)	8.60E+01	3.20E+01		4.40E+01	1.80E+01	
	m (g)	8.60E+01	3.04E+02	→	2.64E+02	1.26E+02	
synthesis 2a	**m scale-up (g)**	*2.11E+01*			*1.08E+01*		
synthesis 3	**m scale-up (g)**	*1.74E+02*			*5.35E+02*		
synthesis 6	**m scale-up (g)**	*2.18E+01*			*6.69E+01*		
	Dichloromethane	**CCl_2H_2**	**O_2**		**CO_2**	**HCl**	
	n mol	1	1		1	2	
	MM (g/mol)	8.49E+01	3.20E+01	→	4.40E+01	3.65E+01	
	m (g)	8.49E+01	3.20E+01		4.40E+01	7.29E+01	
synthesis 4	**m scale-up (g)**	*1.03E+01*			*5.35E+00*	*8.86E+00*	
synthesis 5	**m scale-up (g)**	*3.01E+02*			*1.56E+02*	*2.58E+02*	
	N,N dimethyl formamide	**C_3H_7NO**	**O_2**		**CO_2**	**H_2O**	**NO_2**
	n mol	2	10.5		6	7	2
	MM (g/mol)	7.31E+01	3.20E+01	→	4.40E+01	1.80E+01	4.60E+01
	m (g)	1.46E+02	3.36E+02		2.64E+02	1.26E+02	9.20E+01
synthesis 6.1	**m scale-up (g)**	*7.53E+01*			*1.36E+02*		*4.74E+01*

S3. Empirical estimation of the heat capacities

The temperature dependence model provided by Xia et al. [10] was used to estimate the heat capacities, as a function of the temperature, of the majority of the organic compounds involved in the syntheses. For each compound, the parameters of the empirical polynomial equation (Eq. S2) were estimated by multiplying the number and kind of elements and chemical bonds in the compound by the contribution values provided by Xia et al. In Table S25 the parameters of the empirical polynomial equation, the reaction temperature and the estimated heat capacities are reported.

Equation S2: $C_{pl}(T) = A + BT + CT^2 + DT^3$

where $C_{pl}(T)$ is the heat capacity of liquids as a function of the temperature in J/(mol*K), A, B, C and D are empirical parameters and T is the reaction temperature in K.

For the compounds where it was not possible to use the temperature dependence model, due to the lack of contribution values in Xia et al. for certain bonds present in the molecule, other sources were used and are reported in Table S26.

Table S25. Empirical parameters of the temperature dependence model, reaction temperature and heat capacities of liquids.

Name	***A***	***B***	***C***	***D***	***T*** **[K]**	***C_{pl} (T)*** **[J/(kg*K)]**
Benzoyl chloride	4.69	1.21	-2.63E-03	2.34E-06	333.15	1.44E+03
Cyclohexene	94.6	0.422	-1.26E-03	1.95E-06	333.15	2.04E+03
Cyclohexane	109	0.347	-1.10E-03	1.87E-06	298.15	1.95E+03
Butanol	40.4	0.930	-2.45E-03	2.95E-06	353.15	2.61E+03
Bromobutane	115	0.304	-1.04E-03	1.79E-06	355.15	1.25E+03
Urea	-139	1.88	-4.42E-03	4.01E-06	298.15	2.26E+03
Tributylammine	325	0.588	-1.83E-03	2.89E-06	355.15	2.33E+03
Cyclohexylphenylketone	89.3	1.37	-2.59E-03	2.05E-06	333.15	1.78E+03
1-Chloro Cyclohexyl phenyl ketone	88.3	1.51	-2.78E-03	1.98E-06	363.15	1.55E+03
Tetrabutyl ammonium hydroxide[1]	356	1.59	-3.59E-03	3.66E-06	308.15	2.34E+03

1-Bromo Cyclohexyl phenyl ketone	96.0	1.44	-2.48E-03	1.54E-06	353.15	1.30E+03
Cyclohexanone	41.1	0.822	-1.97E-03	2.26E-06	323.15	1.81E+03
Trichloromethylbenzene	71.2	1.016	-2.15E-03	1.80E-06	323.15	1.21E+03
[1] As an approximation, the contribution values for the covalent N-O bond were used in place of the ionic bond.						

Table S26. Reaction temperature and heat capacities of liquids estimated without the temperature dependence model.

Name	*T* [K]	C_{pl} *(T)* [J/(kg*K)]	Source
Tetrabutylammoniumbromide	363.15	1.55E+03	Linear regression of the experimental value provided at different temperatures by Burns J.A. and Verrall R.E., (1974) [11]
Di-tert-butyl peroxide	323.15	2.03E+03	Empirical equation provided by Ribeiro da Silva. (2001) [12]

S4. Estimation of the energy consumption for the Advanced Process Calculation (APC) scenario

General assumptions:

The framework and the reference equations were adapted from Diogo et al. [12] The heat capacities (C_p) of the mixtures were calculated as the weighted average of the component C_p values, based on the mixture composition. The same approach was applied to densities (ρ_{mix}). The C_p values used were drawn from freely available online databases, and the corresponding sources are reported in the dedicated sections. When C_p related to the reaction temperature was unavailable, specific values were calculated by linear interpolation of the values provided on the websites. When no data related to the substance were available in the literature, they were estimated empirically following the approach proposed by Xia et al. [10] The procedure for calculating the C_p values is described in detail in chapter S3 of the ESI.

Synthesis 1

The steps of the reaction are described in chapter S1. The flows estimated for the upscaling of the APC scenario are reported in Table S10 (Step 1) and Table S11 (Step 2). The C_p of CPK has been estimated according to the framework reported in chapter S3.

Table S27. Stirring and heating energy flows estimated for the reaction occurring in Step 1 of the synthesis 1.

STEP 1								
Inputs	**Mass (kg)**	**Mass (%)**	**Blending**			**Heat**		
Cyclohexyl phenylketone	9.22E+02	72.6%	**E_{stir}**	1.91E-04	MJ	**Q_{react}**	1.29E+03	MJ
Chlorine (gas)	3.47E+02	27.4%	**E_{stir}**	1.91E+02	J	η_{HEAT}	7.50E-01	/
Electricity	**1.76E-04**	**MJ**	Np	3.44E+00	/	Q_{heat}	1.22E+02	MJ
Heat	**1.94E+01**	**MJ**	pmix	8.62E-01	pmix	C_p	1.75E+03	J/kg*K
			N^3	1.49E+00	1/s	m_{mix}	1.00E+03	kg
			d^5	7.22E-03	m	T_r	3.43E+02	K
			time	5.40E+03	s	T_0	2.73E+02	K
			nstir	9.00E-01	/	Q_{loss}	1.25E+03	MJ
						Q_{loss}	1.25E+09	W/s (=J)
						A	5.90E+03	m^2
						k_a/s	5.60E-01	$W/(m^2*k)$
						T_r	3.43E+02	K
						T_{out}	2.73E+02	K
						time	5.40E+03	s

The C_p of Cl-CPK and TBA-Br has been estimated according to the framework reported in chapter S3. The C_p of NaOH was estimated in accordance with the data reported on the NIST website [13].

Table S28. Stirring and heating energy flows estimated for the reaction occurring in Step 2 of the synthesis 1.

STEP 2

Inputs	Mass (kg)	Mass (%)
1-chlorocyclohexyl phenyl ketone	1.09E+03	77.7%
NaOH	3.06E+02	21.8%
Tetrabutylammonium bromide	7.35E+00	0.5%
Electricity (blending)	**6.52E-03**	**MJ**
Heat	**2.92E+03**	**MJ**

	Cp (J/kg*K)
1-chlorocyclohexyl benzophenone	2.00E+03
NaOH	3.82E+02
Tetrabutylammonium bromide	1.73E+03

Blending			Heat		
E_{stir}	8.86E-04	MJ	Q_{react}	2.08E+03	MJ
E_{stir}	8.86E+02	J	η_{HEAT}	7.70E-01	/
Np	3.44E+00	/	Q_{heat}	1.48E+02	MJ
pmix	1.33E+00	pmix	C_p	1.65E+03	J/kg*K
N^3	1.49E+00	1/s	m_{mix}	1.00E+03	kg
d^5	7.22E-03	m	T_r	3.63E+02	K
time	1.62E+04	s	T_0	2.73E+02	K
nstir	9.00E-01	/	Q_{loss}	4.82E+03	MJ
			Q_{loss}	4.82E+09	W/s (=J)
			A	5.90E+03	m^2
			k_a/s	5.60E-01	W/(m^2*k)
			T_r	3.63E+02	K
			T_{out}	2.73E+02	K
			time	1.62E+04	s

Synthesis 2

The steps of the reaction are described in chapter S1. The first step of synthesis 2 is the same as synthesis 1 (Table S10). The second step is reported in Table S12. The C_p of Cl-CPK and TBA-OH have been estimated according to the framework reported in chapter S3. The C_p of dichloroethane was estimated in accordance with the data reported on the NIST website [13]. The C_p of petroleum ether was estimated in accordance with the data reported on The Engineering toolbox (2025) [14].

Table S29. Stirring and heating energy flows estimated for the reaction occurring in Step 1 of the synthesis 2.

STEP 1

Inputs	Mass (kg)	Mass (%)
1-chlorocyclohexyl phenyl ketone	1.17E+03	16%
Dichloroethane	3.29E+03	44%
tetrabutylammonium hydroxide	1.64E+03	22%
Petroleoum ether	1.37E+03	18%
Electricity	**1.91E-03**	**MJ**
Heat	**2.76E+03**	**MJ**

	Cp (J/kg*K)
1-chlorocyclohexyl phenyl ketone	1.54E+03
Dichloroethane	1.20E+03
tetrabutylammonium hydroxide	2.34E+03
Petroleoum ether	1.76E+03

Blending		
$\mathbf{E_{stir}}$	2.55E-04	MJ
$\mathbf{E_{stir}}$	2.55E+02	J
Np	3.44E+00	/
pmix	1.15E+00	pmix
N^3	1.49E+00	1/s
d^5	7.22E-03	m
time	5.40E+03	s
nstir	9.00E-01	/

Heat		
Q_{react}	3.70E+02	MJ
η_{HEAT}	7.50E-01	/
Q_{heat}	5.62E+01	MJ
C_p	1.61E+03	J/kg*K
m_{mix}	1.00E+03	kg
T_r	3.08E+02	K
T_0	2.73E+02	K
Q_{loss}	6.24E+02	MJ
Q_{loss}	6.24E+08	W/s (=J)
A	5.90E+03	m^2
k_a/s	5.60E-01	$W/(m^2*k)$
T_r	3.08E+02	K
T_{out}	2.73E+02	K
time	5.40E+03	s

Synthesis 3

The steps of the reaction are described in chapter S1. The flows estimated for the upscaling of the APC scenario are reported in Table S13 (Step 1) and Table S14 (Step 2). The C_p of Br-CPK has been estimated according to the framework reported in chapter S3. The C_p of NaOH was estimated in accordance with the data reported on the NIST website [13].

Table S30. Stirring and heating energy flows estimated for the reaction occurring in Step 1 of the synthesis 3.

STEP 1

Inputs	**Mass (kg)**	**Mass (%)**
1-bromo-cyclohexyl-phenylketone	2.20E+03	52.4%
NaOH	2.00E+03	47.6%
Electricity	**9.44E-04**	**MJ**
Heat	**-5.01E+03**	**MJ**

	Cp (J/kg*K)
1-bromo-cyclohexyl-phenylketone	1.30E+03
NaOH	1.57E+03

E_{stir}	**2.25E-04**	MJ
E_{stir}	2.25E+02	J
Np	3.44E+00	/
pmix	1.52E+00	pmix
N^3	1.49E+00	1/s
d^5	7.22E-03	m
time	3.60E+03	s
nstir	9.00E-01	/

Q_{react}	**-1.19E+03**	MJ
η_{HEAT}	7.50E-01	/
Q_{heat}	1.14E+02	MJ
C_p	1.43E+03	J/kg*K
m_{mix}	1.00E+03	kg
T_r	3.53E+02	K
T_0	2.73E+02	K
Q_{loss}	9.51E+02	MJ
Q_{loss}	9.51E+08	W/s (=J)
A	5.90E+03	m^2
k_a/s	5.60E-01	$W/(m^2*k)$
T_r	3.53E+02	K
T_{out}	2.73E+02	K
time	3.60E+03	s

Table S31. Stirring energy flows estimated for the reaction occurring in Step 2 of the synthesis 3.

STEP 2

Inputs	**Mass (kg)**	**Mass (%)**
1-hydroxycyclohexyl phenyl ketone	1.00E+03	4.6%
Water	3.33E+03	15.3%
HCl	3.31E-01	0.0%
Petroleum ether	1.74E+04	80.1%
Electricity	**3.63E-04**	**MJ**

E_{stir}	1.67E-05	MJ
E_{stir}	1.67E+01	J
Np	3.44E+00	/
pmix	6.77E-01	pmix
N^3	1.49E+00	1/s
d^5	7.22E-03	m
time	6.00E+02	s
nstir	9.00E-01	/

Synthesis 4

The steps of the reaction are described in chapter 1. The flows estimated for the upscaling of the APC scenario are reported in Table S15 (Step 1) and Table S16 (Step 2). The C_p of CPK, carbon tetrachloride and TBA-Br have been estimated according to the framework reported in chapter S3.

Table S32. Stirring and heating energy flows estimated for the reaction occurring in Step 1 of the synthesis 4.

STEP 1

Inputs	Mass (kg)	Mass (%)
Crude cyclohexyl phenyl ketone	9.22E+02	37.2%
Tetrabutylammonium bromide	2.77E+01	1.1%
Carbon tetrachloride	1.14E+03	45.8%
Sodium hydroxide	3.92E+02	15.8%
Electricity	**6.47E-03**	**MJ**
Heat	**3.90E+04**	**MJ**

E_{stir}	2.61E-03	MJ	**Q_{react}**	**1.57E+04**	MJ
E_{stir}	2.61E+03	J	η_{HEAT}	7.50E-01	/
Np	3.44E+00	/	Q_{heat}	1.10E+02	MJ
pmix	1.47E+00	pmix	C_p	1.30E+03	J/kg*K
N^3	1.49E+00	1/s	m_{mix}	1.00E+03	kg
d^5	7.22E-03	m	T_r	3.58E+02	K
time	4.32E+04	s	T_0	2.73E+02	K
nstir	9.00E-01	/	Q_{loss}	1.21E+04	MJ
			Q_{loss}	1.21E+10	W/s (=J)
			A	5.90E+03	m^2
			k_a/s	5.60E-01	$W/(m^2*k)$
			T_r	3.58E+02	K
			T_{out}	2.73E+02	K
			time	4.32E+04	s

	Cp (J/kg*K)
Cyclohexylphenylketone	1.71E+03
Tetrabutylammonium bromide	1.73E+03
Carbon tetrachloride	8.54E+02
Sodium hydroxide	1.57E+03

Table S33. Stirring energy flows estimated for the reaction occurring in Step 2 of the synthesis 4.

STEP 2

Inputs	Mass (kg)	
Dichloro methane	1.03E+03	
Saturated brine	9.33E+02	
Hydroxycyclohexylphenylketone	1.00E+03	
Electricity	**5.48E-03**	**MJ**

E_{stir}	1.85E-03	MJ
E_{stir}	1.85E+03	J
Np	3.44E+00	/
pmix	1.25E+00	pmix
N^3	1.49E+00	1/s
d^5	7.22E-03	m
time	3.60E+04	s
nstir	9.00E-01	/

Synthesis 5

The steps of the reaction are described in chapter 1. The flows estimated for the upscaling of the APC scenario are reported in Table S17 (Step 1) and Table S18 (Step 2). The C_p of CPK, and Di-tert-butyl peroxide. The C_p of DCM was estimated in accordance with the data reported on the NIST website[13].

Table S34. Stirring and heating energy flows estimated for the reaction occurring in Step 1 of the synthesis 5.

STEP 1

Inputs	Mass (kg)	Mass (%)
Cyclohexyl phenyl ketone	1.06E+03	26.8%
Di-tert-butyl peroxide	2.61E+03	65.7%
Dichloromethane	3.01E+02	7.6%
Electricity	**6.63E-05**	**MJ**
Heat	**1.02E+03**	**MJ**

	Cp (J/kg*K)
Cyclohexyl phenyl ketone	1.71E+03
Di-tert-butyl peroxide	2.03E+03
Dichloromethane	1.04E+03

E_{stir}	1.67E-05	MJ
E_{stir}	1.67E+01	J
Np	3.44E+00	/
pmix	6.77E-01	pmix
N^3	1.49E+00	1/s
d^5	7.22E-03	m
time	6.00E+02	s
nstir	9.00E-01	/

Q_{react}	2.57E+02	MJ
η_{HEAT}	7.50E-01	/
Q_{heat}	9.34E+01	MJ
C_p	1.87E+03	J/kg*K
m_{mix}	1.00E+03	kg
T_r	3.23E+02	K
T_0	2.73E+02	K
Q_{loss}	9.91E+01	MJ
Q_{loss}	9.91E+07	W/s (=J)
A	5.90E+03	m^2
k_a/s	5.60E-01	$W/(m^2*k)$
T_r	3.23E+02	K
T_{out}	2.73E+02	K
time	6.00E+02	s

Table S35. Stirring and heating energy flows estimated for the reaction occurring in Step 2 of the synthesis 5.

STEP 2

Inputs	Mass (kg)	Mass (%)
Sodium hydrogen sulfite	2.12E+03	66.9%
Water	4.92E+00	0.2%
Hydroxycyclohexylphenylketone	1.04E+03	32.9%

E_{stir}	1.34E-04	MJ
E_{stir}	1.34E+02	J
Np	3.44E+00	/
pmix	9.07E-01	pmix

Electricity	**4.24E-04**	**MJ**

N^3	1.49E+00	1/s
d^5	7.22E-03	m
time	3.60E+03	s
nstir	9.00E-01	/

Synthesis 6

The steps of the reaction are described in chapter S1. The flows estimated for the upscaling of the APC scenario are reported in Table S19 (Step 1) and Table S20 (Step 2). The C_p of Magnesium powder, Dymethylformamide, Cyclohexanone and Trichloromethylbenzene have been estimated according to the framework reported in chapter S3. The C_p of petroleum ether was estimated in accordance with the data reported on The Engineering toolbox (2025)[14]

Table S36. Stirring and heating energy flows estimated for the reaction occurring in Step 1 of the synthesis 6.

STEP 1								
Inputs	**Mass (kg)**	**Mass (%)**	**E_{stir}**	2.46E-04	MJ	Q_{react}	-1.56E+03	MJ
Magnesium powder	6.45E+02	**6%**	**E_{stir}**	2.46E+02	J	η_{HEAT}	7.70E-01	/
Dimethylformamide	5.38E+03	**54%**	Np	3.44E+00	/	Q_{heat}	9.36E+01	MJ
Cyclohexanone	5.27E+02	**5%**	pmix	1.11E+00	pmix	C_p	1.87E+03	J/kg*K
Trichloromethylbenzene	1.26E+03	**13%**	N^3	1.49E+00	1/s	m_{mix}	1.00E+03	kg
Dimethylformamide	2.15E+03	**22%**	d^5	7.22E-03	m	T_r	3.23E+02	K
Electricity	**2.45E-03**	**MJ**	time	5.40E+03	s	T_0	2.73E+02	K
Heat	**-1.55E+04**	**MJ**	nstir	9.00E-01	/	Q_{loss}	1.98E+01	MJ
						Q_{loss}	1.98E+07	W/s (=J)
						A	5.90E+03	m^2
						k_a/s	5.60E-01	W/(m^2*k)
						T_r	3.23E+02	K
						T_{out}	2.73E+02	K
						time	1.20E+02	s

	Cp (J/kg*K)
Magnesium powder	1.04E+03
Dimethylformamide	2.06E+03
Cyclohexanone	1.81E+03
Trichloromethylbenzene	1.21E+03
Dimethylformamide	2.06E+03

The C_p of HCPK have been estimated according to the framework reported in chapter S3.

Table S37. Stirring and heating energy flows estimated for the reaction occurring in Step 2 of the synthesis 6.

STEP 2

In	Mass (kg)	Mass (%)
Petroleum ether	9.90E+01	**73.3%**
NaOH 30%	2.00E+01	**14.8%**
HCPK	1.60E+01	**11.9%**
Electricity	**1.17E-05**	**MJ**
Heat	**-2.79E+01**	**MJ**

	Cp (J/kg*K)
Petroleum ether	1.76E+03
NaOH 30%	4.71E+02
Hydroxycyclohexylphenylketone	1.78E+03

E_{stir}	9.85E-05	MJ	**Q_{react}**	-1.22E+03	MJ
E_{stir}	9.85E+01	J	η_{HEAT}	7.70E-01	/
Np	3.44E+00	/	Q_{heat}	7.86E+01	MJ
pmix	1.33E+00	pmix	C_p	1.57E+03	J/kg*K
N^3	1.49E+00	1/s	m_{mix}	1.00E+03	kg
d^5	7.22E-03	m	T_r	3.23E+02	K
time	1.80E+03	s	T_0	2.73E+02	K
nstir	9.00E-01	/	Q_{loss}	2.97E+02	MJ
			Q_{loss}	2.97E+08	W/s (=J)
			A	5.90E+03	m^2
			k_a/s	5.60E-01	W/(m^2*k)
			T_r	3.23E+02	K
			T_{out}	2.73E+02	K
			time	1.80E+03	s

S5. Estimation of the energy consumption for the Software-assisted modelling (SAM) scenario

General assumptions:

Several organic species involved in the synthesis processes, including Br-CPK, CPK, Cl-CPK, HCPK, TBA-Br, and TBA-OH, are not available in the standard Aspen Plus thermodynamic databases. Consequently, these compounds were explicitly defined based on their molecular structures, specifying atomic connectivity and corresponding functional groups. From this structural representation, the software automatically estimated the required physicochemical properties, such as critical constants, heat capacities, and equilibrium properties, using group contribution methods. All reaction stages were modelled using Gibbs reactors to represent thermodynamic equilibrium. It was assumed that the catalytic and phase-transfer agents (e.g., TBA-Br, TBA-OH, benzyl-triethylammonium chloride) were not consumed during the reactions; therefore, their mass input and output flows were kept constant. Likewise, magnesium powder was considered a catalytic species and was not consumed stoichiometrically. Liquid-liquid extractions were simulated using ideal separator blocks, assuming complete phase separation and the absence of chemical reactions in the subsequent units. Petroleum ether, used in extraction steps, was represented as pure hexane to simplify the model, and brine streams were approximated as a binary mixture of water and sodium chloride. Heaters and coolers were modelled as isothermal units operating at specified temperatures, while pressure effects were neglected and atmospheric pressure was assumed throughout. The mass flow rates of all feed streams were taken from APC data, and operating conditions were applied according to the specifications of each synthesis route. After convergence of the simulations, in cases where the reagent was in excess, the feed was adjusted to include only the amount consumed in the reaction, optimising the raw materials used and, therefore, the process. The results were then normalised to 1 kg of HCPK and used to perform the LCA of each synthesis pathway (see Table S1-S6).

Synthesis 1

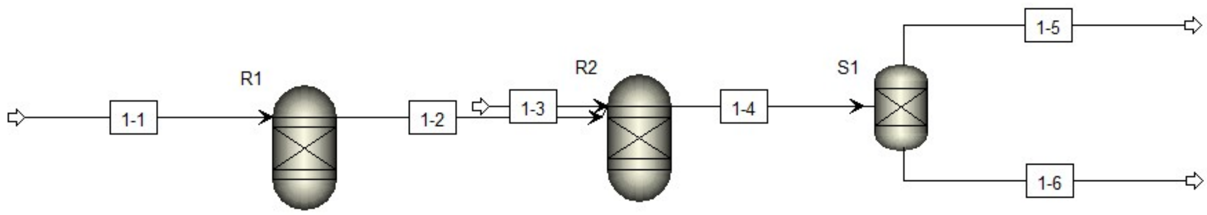


Fig. S10. Flowsheet of the process simulated in ASPEN PLUS software to obtain HCPK through synthesis 1.

Synthesis 2

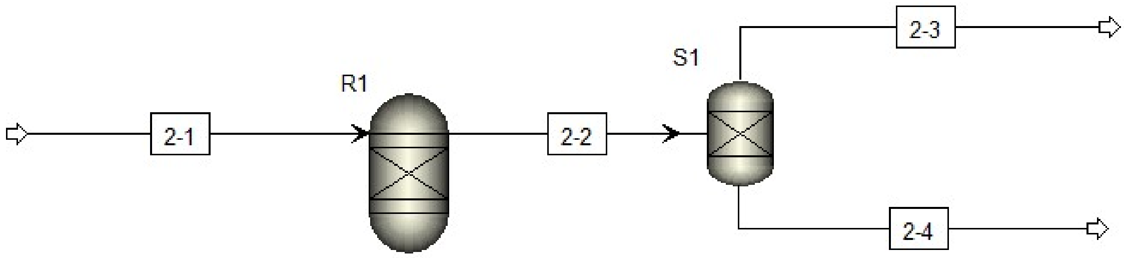


Fig. S11. Flowsheet of the process simulated in ASPEN PLUS software to obtain HCPK through synthesis 2.

Synthesis 3

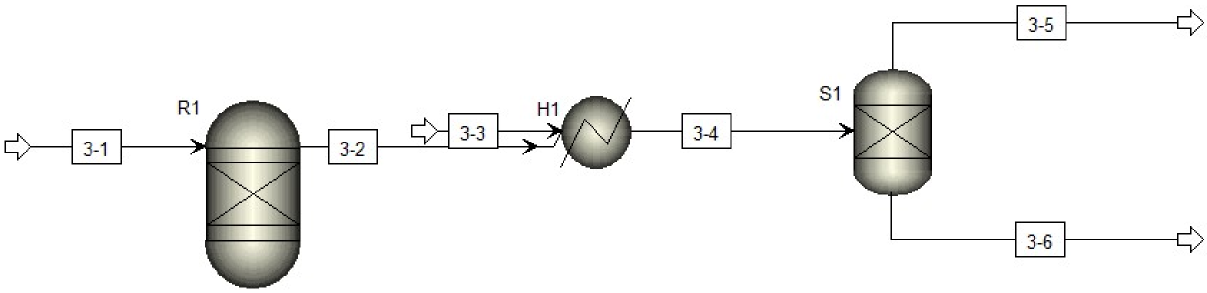


Fig. S12. Flowsheet of the process simulated in ASPEN PLUS software to obtain HCPK through synthesis 3.

Synthesis 4

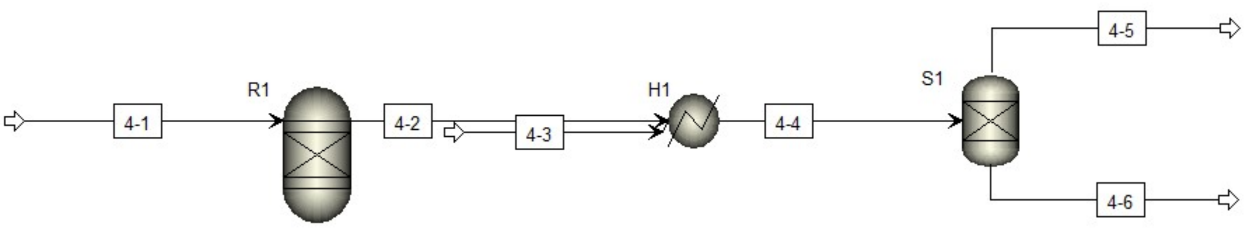


Fig. S13. Flowsheet of the process simulated in ASPEN PLUS software to obtain HCPK through synthesis 4.

Synthesis 5

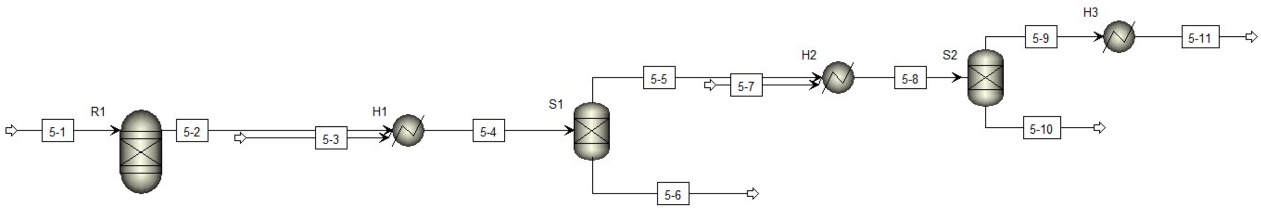


Fig. S14. Flowsheet of the process simulated in ASPEN PLUS software to obtain HCPK through synthesis 5.

Synthesis 6

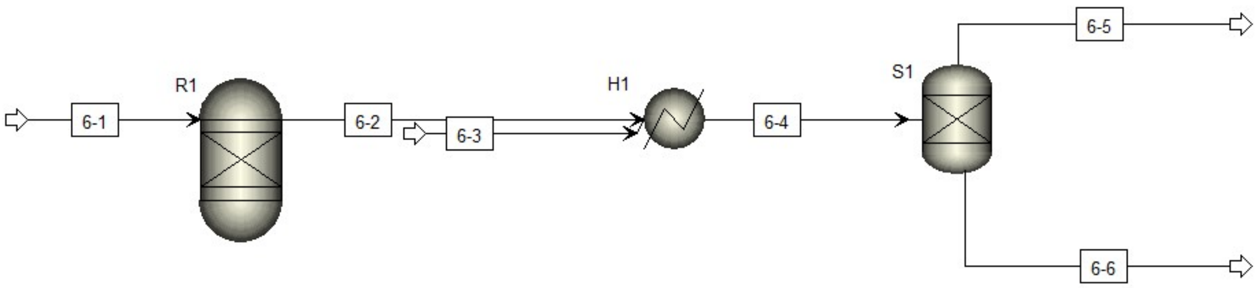


Fig. S15. Flowsheet of the process simulated in ASPEN PLUS software to obtain HCPK through synthesis 6.

S7. Statistical treatment

Table S38. Uncertainty factors and standard deviations from Pedigree matrix approach [15]

	Reagents and solvents Lab scale	Reagents and solvents APC	Reagents and solvents ASPEN	Electricity lab scale	Electricity, heat & cooling ASPEN	Reaxys	Energy APC	Waste	Emissions
U1 (reliability)	1.00	1.20	1.10	1.05	1.05	1.10	1.10	1.05	1.20
U2 (completeness)	1.00	1.00	1.00	1.02	1.00	1.05	1.00	1.00	1.00
U3 (temporal c.)	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
U4 (geographical c.)	1.00	1.00	1.00	1.00	1.00	1.01	1.00	1.00	1.00
U5 (technological c.)	1.00	1.00	1.00	1.00	1.00	1.20	1.00	1.00	1.00
Ub (basic uncertainty)	1.05	1.05	1.05	1.05	1.05	1.05	1.05	1.05	1.05
SD	1.05E+00	1.21E+00	1.11E+00	1.07E+00	1.07E+00	1.24E+00	1.11E+00	1.07E+00	1.21E+00

S8. Life Cycle Assessment Results

Table S39. Life Cycle Impact Assessment results of synthesis 1, Lab Scale scenario.

			AC (mol H^+ eq)	CC (kg CO_2 eq)	ECOTOX (CTUe)	PM (kg PM 2.5)	MEU (kg N eq)	FEU (kg P eq)	TEU (mol N eq)	HTOX_c (CTUh)	HTOX_nc (CTUh)
S1	Step 1	CPK	2.5E-02	7.6E+00	2.8E+02	2.8E-07	4.7E-03	1.7E-03	4.8E-02	9.7E-09	5.1E-08
		Chlorine (gas)	9.3E-04	2.0E-01	2.3E+00	7.2E-09	2.0E-04	1.6E-04	1.8E-03	1.6E-09	2.6E-09
		Electricity	1.7E-02	4.8E+00	1.5E+01	1.0E-07	3.5E-03	9.8E-04	3.4E-02	1.1E-08	3.1E-08
		HCl	1.3E-04	2.5E-01	1.9E+00	2.0E-09	5.2E-05	3.6E-05	4.4E-04	6.0E-11	2.0E-10
	Step 2	NaOH	2.3E-03	4.1E-01	3.1E+00	2.2E-08	4.8E-04	2.0E-04	4.8E-03	2.2E-09	5.8E-09
		TBA-Br	4.2E-04	1.8E-01	4.9E-01	4.5E-09	8.0E-05	2.4E-05	8.3E-04	7.3E-11	6.1E-10
		Electricity	4.6E-03	1.3E+00	4.0E+00	2.7E-08	9.6E-04	2.7E-04	9.2E-03	3.0E-09	8.4E-09
		NaCl	4.3E-04	8.4E-01	6.4E+00	6.8E-09	1.8E-04	1.2E-04	1.5E-03	2.0E-10	6.8E-10
	Total		***5.0E-02***	***1.6E+01***	***3.1E+02***	***4.5E-07***	***1.0E-02***	***3.5E-03***	***1.0E-01***	***2.8E-08***	***1.0E-07***
	SD%		*9.03%*	*8.24%*	*>100%*	*40.26%*	*9.17%*	*9.68%*	*>100%*	*>100%*	*64.65%*

			IR (kg U^{235} eq)	LU (Pts)	ODP (kg CFC-11 eq)	POF (kg NMVOC eq)	FRD (MJ)	MRD (kg Sb eq)	WU (m^3)	SS (µp)
S1	Step 1	CPK	3.0E-01	1.7E+01	2.4E-07	2.8E-02	1.4E+02	4.5E-05	1.3E+00	7.2E+02
		Chlorine (gas)	5.6E-02	8.5E-01	1.1E-08	5.4E-04	3.3E+00	2.9E-06	6.8E-02	2.4E+01
		Electricity	1.2E+00	4.9E+01	1.9E-08	1.3E-02	7.8E+01	1.8E-05	4.8E+00	4.1E+02
		HCl	1.8E-03	6.8E-02	7.8E-10	1.3E-04	3.7E-01	1.1E-07	7.0E-03	9.8E-03
	Step 2	NaOH	4.8E-02	1.4E+00	5.4E-08	1.4E-03	5.4E+00	3.9E-06	2.3E-01	4.3E-02
		TBA-Br	3.6E-03	1.8E-01	4.6E-09	3.9E-04	2.4E+00	4.0E-07	3.6E-02	1.1E-02
		Electricity	3.3E-01	1.3E+01	5.0E-09	3.7E-03	2.1E+01	4.8E-06	1.3E+00	1.1E+02
		NaCl	6.1E-03	2.3E-01	2.6E-09	4.5E-04	1.3E+00	3.6E-07	2.4E-02	3.3E-02
	Total		***1.9E+00***	***8.2E+01***	***3.3E-07***	***4.8E-02***	***2.5E+02***	***7.5E-05***	***7.7E+00***	***1.3E+03***
	SD%		*15.71%*	*15.63%*	*21.34%*	*12.73%*	*9.92%*	*30.56%*	*>100%*	*/*

Table S40. Life Cycle Impact Assessment results of synthesis 2, Lab Scale scenario.

			AC (mol H^+ eq)	**CC** (kg CO_2 eq)	**ECOTOX** (CTUe)	**PM** (kg PM 2.5)	**MEU** (kg N eq)	**FEU** (kg P eq)	**TEU** (mol N eq)	**HTOX_c** (CTUh)	**HTOX_nc** (CTUh)
S2	**Step 1**	CPK	2.6E-02	8.0E+00	2.9E+02	2.9E-07	4.9E-03	1.8E-03	5.1E-02	1.0E-08	5.4E-08
		Chlorine (gas)	9.8E-04	2.1E-01	2.4E+00	7.6E-09	2.1E-04	1.7E-04	1.9E-03	1.7E-09	2.8E-09
		Electricity	1.8E-02	5.1E+00	1.6E+01	1.1E-07	3.7E-03	1.0E-03	3.6E-02	1.2E-08	3.3E-08
		HCl	1.3E-04	2.6E-01	2.0E+00	2.1E-09	5.5E-05	3.8E-05	4.6E-04	6.3E-11	2.1E-10
	Step 2	Dichloroethane	1.6E-02	4.5E+00	2.8E+01	1.2E-07	3.4E-03	1.9E-03	3.2E-02	1.8E-08	5.3E-08
		TBA-OH	1.2E-01	5.1E+01	1.8E+02	1.3E-06	2.4E-02	7.4E-03	2.5E-01	2.7E-08	1.9E-07
		Petroleum ether	4.9E-03	1.1E+00	4.2E+00	4.5E-08	8.6E-04	1.6E-04	9.3E-03	2.3E-10	1.0E-08
		Electricity	1.1E-02	3.1E+00	9.5E+00	6.4E-08	2.3E-03	6.3E-04	2.2E-02	6.9E-09	2.0E-08
		Waste	1.8E-03	3.6E+00	2.7E+01	2.9E-08	7.5E-04	5.2E-04	6.3E-03	8.6E-10	2.9E-09
		CO_2	0.0E+00	7.7E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
		HCl	0.0E+00	0.0E+00	6.1E+01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
	Total		***2.0E-01***	***8.4E+01***	***6.3E+02***	***2.0E-06***	***4.0E-02***	***1.4E-02***	***4.1E-01***	***7.6E-08***	***3.6E-07***
	SD%		14.90%	14.47%	>100%	46.46%	13.97%	13.93%	>100%	>100%	60.26%

			IR (kg U^{235} eq)	**LU** (Pts)	**ODP** (kg CFC-11 eq)	**POF** (kg NMVOC eq)	**FRD** (MJ)	**MRD** (kg Sb eq)	**WU** (m^3)	**SS** (µp)
S2	**Step 1**	CPK	3.2E-01	1.8E+01	2.5E-07	2.9E-02	1.5E+02	4.8E-05	1.4E+00	7.6E+02
		Chlorine (gas)	5.9E-02	9.0E-01	1.2E-08	5.7E-04	3.5E+00	3.1E-06	7.2E-02	2.5E+01
		Electricity	1.3E+00	5.1E+01	2.0E-08	1.4E-02	8.3E+01	1.9E-05	5.0E+00	4.4E+02
		HCl	1.9E-03	7.2E-02	8.2E-10	1.4E-04	4.0E-01	1.1E-07	7.4E-03	1.0E-02
	Step 2	Dichloroethane	7.1E-01	1.4E+01	2.2E-07	3.0E-02	1.1E+02	5.4E-05	1.3E+00	5.0E+02
		TBA-OH	1.1E+00	5.7E+01	1.3E-06	1.1E-01	6.7E+02	1.2E-04	1.0E+01	3.3E+00
		Petroleum ether	2.4E-02	4.7E+00	6.7E-08	1.1E-02	5.4E+01	8.4E-06	4.9E-01	1.5E-01
		Electricity	7.7E-01	3.1E+01	1.2E-08	8.6E-03	5.0E+01	1.1E-05	3.0E+00	2.6E+02
		Waste	2.6E-02	9.8E-01	1.1E-08	1.9E-03	5.4E+00	1.5E-06	1.0E-01	1.4E-01
		CO_2	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	2.2E+02
		HCl	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	2.1E+01
	Total		***4.3E+00***	***1.8E+02***	***1.9E-06***	***2.1E-01***	***1.1E+03***	***2.7E-04***	***2.2E+01***	***2.2E+03***
	SD%		17.31%	25.00%	21.73%	18.26%	15.20%	44.81%	>100%	/

Table S41. Life Cycle Impact Assessment results of synthesis 3, Lab Scale scenario.

			AC (mol H^+ eq)	CC (kg CO_2 eq)	ECOTOX (CTUe)	PM (kg PM 2.5)	MEU (kg N eq)	FEU (kg P eq)	TEU (mol N eq)	HTOX_c (CTUh)	HTOX_nc (CTUh)
S3	**Step 1**	Br-CPK	7.0E-02	2.3E+01	4.9E+02	7.9E-07	1.3E-02	4.3E-03	1.3E-01	2.2E-08	1.3E-07
		NaOH	1.5E-02	2.6E+00	2.0E+01	1.4E-07	3.1E-03	1.3E-03	3.1E-02	1.4E-08	3.7E-08
		Electricity	6.0E-03	1.7E+00	5.3E+00	3.6E-08	1.3E-03	3.5E-04	1.2E-02	3.9E-09	1.1E-08
		NaBr	3.2E-03	6.3E+00	4.8E+01	5.1E-08	1.3E-03	9.2E-04	1.1E-02	1.5E-09	5.1E-09
	Step 2	Water	1.4E-05	1.3E-03	1.7E-01	1.1E-10	1.1E-06	5.8E-07	1.1E-05	2.9E-12	1.9E-11
		HCl	1.1E-06	1.9E-04	2.1E-03	7.8E-12	1.8E-07	1.1E-07	1.6E-06	6.9E-13	2.5E-12
		Petroleum ether	6.2E-02	1.4E+01	5.3E+01	5.8E-07	1.1E-02	2.0E-03	1.2E-01	2.9E-09	1.3E-07
		Electricity	7.5E-03	2.1E+00	6.6E+00	4.5E-08	1.6E-03	4.4E-04	1.5E-02	4.8E-09	1.4E-08
		Wastewater	1.6E-06	3.9E-04	1.5E-03	3.9E-11	4.4E-07	1.3E-07	3.9E-06	1.9E-13	4.3E-12
		CO_2	0.0E+00	5.3E+01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
	Total		***1.6E-01***	***1.0E+02***	***6.2E+02***	***1.6E-06***	***3.1E-02***	***9.2E-03***	***3.2E-01***	***4.9E-08***	***3.2E-07***
	SD%		8.20%	6.16%	>100%	44.29%	7.83%	8.19%	>100%	>100%	50.93%

			IR (kg U^{235} eq)	LU (Pts)	ODP (kg CFC-11 eq)	POF (kg NMVOC eq)	FRD (MJ)	MRD (kg Sb eq)	WU (m^3)	SS (µp)
S3	**Step 1**	Br-CPK	7.4E-01	3.9E+01	6.5E-07	6.8E-02	3.6E+02	1.0E-04	2.8E+00	1.9E+03
		NaOH	3.1E-01	8.7E+00	3.5E-07	9.2E-03	3.5E+01	2.5E-05	1.5E+00	2.7E-01
		Electricity	4.3E-01	1.7E+01	6.6E-09	4.8E-03	2.8E+01	6.3E-06	1.7E+00	1.5E+02
		NaBr	4.5E-02	1.7E+00	2.0E-08	3.3E-03	9.5E+00	2.7E-06	1.8E-01	2.5E-01
	Step 2	Water	1.7E-04	5.6E-03	5.1E-10	4.3E-06	1.7E-02	1.7E-08	1.5E-01	1.3E-03
		HCl	4.0E-05	7.2E-04	3.2E-11	5.5E-07	3.3E-03	3.0E-09	9.2E-05	2.2E-05
		Petroleum ether	3.1E-01	5.9E+01	8.5E-07	1.4E-01	6.9E+02	1.1E-04	6.2E+00	1.9E+00
		Electricity	5.4E-01	2.2E+01	8.3E-09	6.0E-03	3.5E+01	7.9E-06	2.1E+00	1.8E+02
		Wastewater	2.8E-05	2.8E-03	2.6E-12	1.2E-06	3.9E-03	2.9E-09	-1.4E-01	-1.0E-06
		CO_2	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1.5E+03
	Total		***2.4E+00***	***1.5E+02***	***1.9E-06***	***2.4E-01***	***1.2E+03***	***2.5E-04***	***1.5E+01***	***3.7E+03***
	SD%		13.09%	10.34%	20.23%	16.87%	9.41%	36.88%	>100%	/

Table S42. Life Cycle Impact Assessment results of synthesis 4, Lab Scale scenario.

			AC (mol H^+ eq)	CC (kg CO_2 eq)	ECOTOX (CTUe)	PM (kg PM 2.5)	MEU (kg N eq)	FEU (kg P eq)	TEU (mol N eq)	HTOX_c (CTUh)	HTOX_nc (CTUh)
S4	Step 1	CPK	2.4E-02	7.5E+00	2.8E+02	2.7E-07	4.6E-03	1.7E-03	4.7E-02	9.6E-09	5.1E-08
		TBA-Br	1.6E-03	6.5E-01	1.8E+00	1.7E-08	3.0E-04	8.8E-05	3.1E-03	2.7E-10	2.3E-09
		Carbon tetrachloride	1.7E-02	1.9E+00	2.2E+01	2.8E-07	3.3E-03	4.4E-05	3.6E-02	6.4E-10	7.4E-08
		NaOH	2.9E-03	5.2E-01	3.9E+00	2.8E-08	6.0E-04	2.5E-04	6.0E-03	2.7E-09	7.3E-09
		Electricity	8.8E-03	2.5E+00	7.7E+00	5.2E-08	1.8E-03	5.1E-04	1.8E-02	5.7E-09	1.6E-08
		Waste	1.5E-03	2.9E+00	2.2E+01	2.3E-08	6.1E-04	4.2E-04	5.1E-03	7.0E-10	2.4E-09
	Step 2	Saturated brine	4.7E-04	6.7E-02	6.4E-01	4.8E-09	1.0E-04	3.7E-05	9.6E-04	3.1E-11	1.5E-09
		Dichloromethane	2.7E-02	3.6E+00	5.8E+01	5.4E-07	5.5E-03	5.3E-05	6.0E-02	5.7E-10	6.6E-08
		Waste	9.4E-04	1.8E+00	1.4E+01	1.5E-08	3.9E-04	2.7E-04	3.2E-03	4.4E-10	1.5E-09
		CO_2	0.0E+00	5.2E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
		HCl	0.0E+00	0.0E+00	1.8E+01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
	Total		***8.5E-02***	***2.2E+01***	***4.2E+02***	***1.2E-06***	***1.7E-02***	***3.3E-03***	***1.8E-01***	***2.1E-08***	***2.2E-07***
	SD%		6.92%	6.62%	>100%	40.82%	8.33%	8.39%	>100%	>100%	45.50%

			IR (kg U^{235} eq)	LU (Pts)	ODP (kg CFC-11 eq)	POF (kg NMVOC eq)	FRD (MJ)	MRD (kg Sb eq)	WU (m^3)	SS (µp)
S4	Step 1	CPK	3.0E-01	1.7E+01	2.3E-07	2.7E-02	1.4E+02	4.4E-05	1.3E+00	7.1E+02
		TBA-Br	1.3E-02	6.7E-01	1.7E-08	1.4E-03	8.8E+00	1.5E-06	1.3E-01	4.2E-02
		Carbon tetrachloride	5.0E-04	1.6E-01	2.4E-10	1.0E-02	3.7E+01	3.7E-07	2.7E+00	2.3E+02
		NaOH	6.0E-02	1.7E+00	6.8E-08	1.8E-03	6.8E+00	4.8E-06	2.9E-01	5.4E-02
		Electricity	6.3E-01	2.5E+01	9.7E-09	7.0E-03	4.1E+01	9.2E-06	2.5E+00	2.1E+02
		Waste	2.1E-02	8.0E-01	9.1E-09	1.5E-03	4.4E+00	1.2E-06	8.2E-02	1.1E-01
	Step 2	Saturated brine	6.2E-03	4.3E-01	8.1E-10	2.9E-04	8.3E-01	2.0E-06	6.2E-02	9.0E-03
		Dichloromethane	5.1E-04	1.3E-01	4.9E-05	1.6E-02	3.9E+01	2.5E-07	4.5E-01	3.9E+02
		Waste	1.3E-02	5.0E-01	5.7E-09	9.7E-04	2.8E+00	7.8E-07	5.2E-02	7.2E-02
		CO_2	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1.4E+01
		HCl	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.1E+00
	Total		***1.0E+00***	***4.7E+01***	***4.9E-05***	***6.7E-02***	***2.8E+02***	***6.5E-05***	***7.6E+00***	***1.6E+03***
	SD%		15.23%	20.86%	9.43%	9.24%	8.56%	39.77%	>100%	/

Table S43. Life Cycle Impact Assessment results of synthesis 5, Lab Scale scenario.

			AC (mol H^+ eq)	CC (kg CO_2 eq)	ECOTOX (CTUe)	PM (kg PM 2.5)	MEU (kg N eq)	FEU (kg P eq)	TEU (mol N eq)	HTOX_c (CTUh)	HTOX_nc (CTUh)
S5	Step 1	CPK	2.8E-02	8.6E+00	3.2E+02	3.1E-07	5.3E-03	1.9E-03	5.5E-02	1.1E-08	5.8E-08
		Di-tert-butyl peroxide	7.4E-02	8.2E+00	4.0E+01	5.0E-07	5.6E-03	1.9E-03	5.4E-02	1.6E-09	4.1E-08
		Dichloromethane	8.3E-03	1.1E+00	1.7E+01	1.6E-07	1.6E-03	1.6E-05	1.8E-02	1.7E-10	2.0E-08
		Electricity	7.4E-03	2.1E+00	6.5E+00	4.4E-08	1.5E-03	4.3E-04	1.5E-02	4.8E-09	1.3E-08
		Waste	2.6E-03	5.2E+00	3.9E+01	4.2E-08	1.1E-03	7.6E-04	9.2E-03	1.2E-09	4.2E-09
		CO_2	0.0E+00	1.6E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
		HCl	0.0E+00	0.0E+00	5.4E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
	Step 2	Sodium hydrogen sulfite	1.0E-01	2.6E+00	3.2E+01	6.7E-07	3.0E-03	1.2E-03	3.1E-02	6.8E-09	4.1E-08
		Water	9.3E-06	8.7E-04	1.1E-01	7.4E-11	7.5E-07	3.8E-07	7.3E-06	1.9E-12	1.3E-11
		Electricity	1.1E-03	3.0E-01	9.3E-01	6.3E-09	2.2E-04	6.1E-05	2.1E-03	6.8E-10	1.9E-09
		Wastewater	1.1E-06	2.6E-04	1.0E-03	2.6E-11	2.9E-07	8.8E-08	2.5E-06	1.3E-13	2.8E-12
		Waste	2.1E-03	4.0E+00	3.0E+01	3.2E-08	8.4E-04	5.9E-04	7.1E-03	9.7E-10	3.3E-09
	Step 3	Water	4.6E-06	4.3E-04	5.5E-02	3.7E-11	3.7E-07	1.9E-07	3.6E-06	9.4E-13	6.2E-12
		Electricity	1.0E-03	2.9E-01	8.8E-01	6.0E-09	2.1E-04	5.8E-05	2.0E-03	6.5E-10	1.8E-09
		Waste	1.1E-03	2.2E+00	1.7E+01	1.8E-08	4.7E-04	3.2E-04	3.9E-03	5.3E-10	1.8E-09
	Total		***2.3E-01***	***3.5E+01***	***5.1E+02***	***1.8E-06***	***2.0E-02***	***7.3E-03***	***2.0E-01***	***2.8E-08***	***1.9E-07***
	SD%		10.31%	7.99%	>100%	26.97%	6.17%	6.48%	>100%	>100%	45.42%

			IR (kg U^{235} eq)	LU (Pts)	ODP (kg CFC-11 eq)	POF (kg NMVOC eq)	FRD (MJ)	MRD (kg Sb eq)	WU (m^3)	SS (μp)
S5	Step 1	CPK	3.4E-01	2.0E+01	2.7E-07	3.1E-02	1.6E+02	5.1E-05	1.5E+00	8.2E+02
		Di-tert-butyl peroxide	1.0E+00	2.9E+01	1.7E-07	2.2E-02	2.0E+02	4.4E-05	1.2E+01	9.0E+02
		Dichloromethane	1.5E-04	4.0E-02	1.5E-05	4.9E-03	1.2E+01	7.6E-08	1.4E-01	1.2E+02
		Electricity	5.3E-01	2.1E+01	8.1E-09	5.9E-03	3.4E+01	7.8E-06	2.1E+00	1.8E+02
		Waste	3.7E-02	1.4E+00	1.6E-08	2.7E-03	7.8E+00	2.2E-06	1.5E-01	2.0E-01
		CO_2	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	4.3E+00
		HCl	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1.8E+00
	Step 2	Sodium hydrogen sulfite	2.9E-01	9.9E+00	1.3E-07	1.5E-02	3.6E+01	6.0E-05	9.7E-01	4.9E-01
		Water	1.1E-04	3.7E-03	3.3E-10	2.8E-06	1.1E-02	1.1E-08	9.7E-02	8.5E-04
		Electricity	7.5E-02	3.0E+00	1.2E-09	8.4E-04	4.9E+00	1.1E-06	3.0E-01	2.6E+01
		Wastewater	1.8E-05	1.9E-03	1.7E-12	8.0E-07	2.5E-03	1.9E-09	-9.4E-02	-6.8E-07
		Waste	2.9E-02	1.1E+00	1.3E-08	2.1E-03	6.1E+00	1.7E-06	1.1E-01	1.6E-01
	Step 3	Water	5.4E-05	1.8E-03	1.7E-10	1.4E-06	5.7E-03	5.7E-09	4.8E-02	4.2E-04
		Electricity	7.2E-02	2.9E+00	1.1E-09	8.0E-04	4.6E+00	1.1E-06	2.8E-01	2.4E+01
		Waste	1.6E-02	6.1E-01	6.9E-09	1.2E-03	3.3E+00	9.5E-07	6.3E-02	8.7E-02

Total	***2.4E+00***	***8.9E+01***	***1.5E-05***	***8.7E-02***	***4.6E+02***	***1.7E-04***	***1.7E+01***	***2.1E+03***	
SD%	11.79%	18.54%	11.07%	9.99%	6.88%	36.54%	>100%	/	

Table S44. Life Cycle Impact Assessment results of synthesis 6, Lab Scale scenario.

			AC (mol H^+ eq)	**CC** (kg CO_2 eq)	**ECOTOX** (CTUe)	**PM** (kg PM 2.5)	**MEU** (kg N eq)	**FEU** (kg P eq)	**TEU** (mol N eq)	**HTOX_c** (CTUh)	**HTOX_nc** (CTUh)
S6	**Step 1**	Benzothrichloride	9.5E-03	2.3E+00	1.4E+01	7.7E-08	1.8E-03	9.6E-04	1.7E-02	8.6E-09	2.1E-08
		N,N dimethyl formamide	1.8E-01	4.1E+01	4.8E+02	2.3E-06	2.5E-02	7.6E-03	5.2E-01	7.7E-09	2.3E-07
		Cyclohexanone	1.0E-02	3.0E+00	2.5E+01	1.1E-07	1.8E-03	5.8E-04	1.9E-02	2.3E-09	2.0E-08
		Electricity	2.3E-02	6.4E+00	2.0E+01	1.3E-07	4.7E-03	1.3E-03	4.5E-02	1.5E-08	4.1E-08
		CO_2	0.0E+00	2.6E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
		NO_2	6.8E-01	0.0E+00	0.0E+00	1.5E-06	3.6E-01	0.0E+00	3.9E+00	0.0E+00	0.0E+00
	Step 2	Petroleoum ether	5.2E-03	1.2E+00	4.4E+00	4.8E-08	9.1E-04	1.7E-04	9.8E-03	2.4E-10	1.1E-08
		NaOH	9.2E-03	1.7E+00	1.2E+01	9.0E-08	1.9E-03	7.9E-04	1.9E-02	8.7E-09	2.3E-08
		Water	5.0E-06	4.6E-04	5.9E-02	3.9E-11	4.0E-07	2.0E-07	3.9E-06	1.0E-12	6.7E-12
		Electricity	1.1E-03	3.0E-01	9.2E-01	6.2E-09	2.2E-04	6.1E-05	2.1E-03	6.8E-10	1.9E-09
		CO_2	0.0E+00	4.5E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
		Wastewater	1.3E-06	3.0E-04	1.2E-03	3.0E-11	3.4E-07	1.0E-07	3.0E-06	1.5E-13	3.3E-12
		Waste	1.3E-03	2.5E+00	1.9E+01	2.0E-08	5.2E-04	3.6E-04	4.3E-03	5.9E-10	2.0E-09
	Total		***9.1E-01***	***6.6E+01***	***5.8E+02***	***4.2E-06***	***3.9E-01***	***1.2E-02***	***4.5E+00***	***4.3E-08***	***3.5E-07***
	SD%		7.38%	4.92%	>100%	41.53%	8.69%	8.33%	>100%	>100%	53.58%
			IR (kg U^{235} eq)	**LU** (Pts)	**ODP** (kg CFC-11 eq)	**POF** (kg NMVOC eq)	**FRD** (MJ)	**MRD** (kg Sb eq)	**WU** (m^3)	**SS** (µp)	
S6	**Step 1**	Benzothrichloride	3.3E-01	7.1E+00	1.4E-07	1.0E-02	6.2E+01	2.0E-05	6.0E-01	2.5E+02	
		N,N dimethyl formamide	8.3E-01	8.5E+01	8.3E-07	1.3E-01	7.4E+02	2.2E-04	1.0E+01	3.6E+00	
		Cyclohexanone	9.7E-02	7.8E+00	8.1E-08	1.3E-02	6.5E+01	2.1E-05	3.4E-01	2.7E+02	
		Electricity	1.6E+00	6.5E+01	2.5E-08	1.8E-02	1.0E+02	2.4E-05	6.4E+00	5.5E+02	
		CO_2	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	7.3E+01	
		NO_2	0.0E+00	0.0E+00	0.0E+00	9.1E-01	0.0E+00	0.0E+00	0.0E+00	3.4E+00	
	Step 2	Petroleoum ether	2.6E-02	5.0E+00	7.0E-08	1.2E-02	5.7E+01	8.9E-06	5.2E-01	1.6E-01	
		NaOH	1.9E-01	5.5E+00	2.2E-07	5.7E-03	2.2E+01	1.5E-05	9.4E-01	1.7E-01	
		Water	5.8E-05	1.9E-03	1.8E-10	1.5E-06	6.1E-03	6.1E-09	5.2E-02	4.5E-04	
		Electricity	7.5E-02	3.0E+00	1.2E-09	8.4E-04	4.8E+00	1.1E-06	3.0E-01	2.6E+01	
		CO_2	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1.2E+02	
		Wastewater	2.2E-05	2.2E-03	2.0E-12	9.5E-07	3.0E-03	2.2E-09	-1.1E-01	-7.9E-07	
		Waste	1.8E-02	6.7E-01	7.7E-09	1.3E-03	3.7E+00	1.0E-06	7.0E-02	9.7E-02	

Total	***3.2E+00***	***1.8E+02***	***1.4E-06***	***1.1E+00***	***1.1E+03***	***3.1E-04***	***1.9E+01***	***1.3E+03***
SD%	16.24%	7.11%	25.06%	8.24%	8.11%	32.27%	>100%	/

Table S45. Life Cycle Impact Assessment results of synthesis 1, APC scenario.

			AC (mol H^+ eq)	**CC** (kg CO_2 eq)	**ECOTOX** (CTUe)	**PM** (kg PM 2.5)	**MEU** (kg N eq)	**FEU** (kg P eq)	**TEU** (mol N eq)	**HTOX_c** (CTUh)	**HTOX_nc** (CTUh)
S1	**Step 1**	CPK	2.5E-02	7.6E+00	2.8E+02	2.8E-07	4.7E-03	1.7E-03	4.8E-02	9.7E-09	5.1E-08
		Chlorine (gas)	9.3E-04	2.0E-01	2.3E+00	7.2E-09	2.0E-04	1.6E-04	1.8E-03	1.6E-09	2.6E-09
		Electricity	7.3E-11	2.1E-08	6.4E-08	4.3E-16	1.5E-11	4.2E-12	1.5E-10	4.7E-17	1.3E-16
		HCl	1.3E-04	2.5E-01	1.9E+00	2.0E-09	5.2E-05	3.6E-05	4.4E-04	6.0E-11	2.0E-10
	Step 2	NaOH	2.3E-03	4.1E-01	3.1E+00	2.2E-08	4.8E-04	2.0E-04	4.8E-03	2.2E-09	5.8E-09
		TBA-Br	4.2E-06	1.7E-03	4.8E-03	4.4E-11	7.9E-07	2.3E-07	8.2E-06	7.2E-13	6.0E-12
		Electricity	3.1E-10	8.7E-08	2.7E-07	1.8E-15	6.4E-11	1.8E-11	6.1E-10	2.0E-16	5.6E-16
		Heat	1.5E-04	1.6E-01	9.6E-02	7.8E-10	4.7E-05	6.2E-06	4.9E-04	3.0E-11	2.9E-10
		NaCl	4.2E-04	8.3E-01	6.3E+00	6.7E-09	1.7E-04	1.2E-04	1.5E-03	2.0E-10	6.7E-10
	Total		***2.9E-02***	***9.4E+00***	***2.9E+02***	***3.2E-07***	***5.6E-03***	***2.2E-03***	***5.7E-02***	***1.4E-08***	***6.1E-08***
	SD%		16.45%	13.65%	>100%	66.49%	15.28%	15.50%	>100%	>100%	>100%

			IR (kg U^{235} eq)	**LU** (Pts)	**ODP** (kg CFC-11 eq)	**POF** (kg NMVOC eq)	**FRD** (MJ)	**MRD** (kg Sb eq)	**WU** (m^3)	**SS** (µp)
S1	**Step 1**	CPK	3.0E-01	1.7E+01	2.4E-07	2.8E-02	1.4E+02	4.5E-05	1.3E+00	7.2E+02
		Chlorine (gas)	5.6E-02	8.5E-01	1.1E-08	5.4E-04	3.3E+00	2.9E-06	6.8E-02	2.4E+01
		Electricity	5.2E-09	2.1E-07	8.0E-17	5.8E-11	3.4E-07	7.7E-14	2.1E-08	1.8E-06
		HCl	1.8E-03	6.8E-02	7.8E-10	1.3E-04	3.7E-01	1.1E-07	7.0E-03	9.8E-03
	Step 2	NaOH	4.8E-02	1.4E+00	5.4E-08	1.4E-03	5.4E+00	3.9E-06	2.3E-01	4.3E-02
		TBA-Br	3.5E-05	1.8E-03	4.5E-11	3.8E-06	2.3E-02	3.9E-09	3.6E-04	1.1E-04
		Electricity	2.2E-08	8.8E-07	3.4E-16	2.4E-10	1.4E-06	3.2E-13	8.6E-08	7.4E-06
		Heat	2.5E-03	6.0E-02	6.2E-09	2.7E-04	2.5E+00	1.7E-07	3.5E-03	8.9E-03
		NaCl	6.0E-03	2.3E-01	2.6E-09	4.4E-04	1.2E+00	3.5E-07	2.3E-02	3.3E-02
	Total		***4.1E-01***	***2.0E+01***	***3.1E-07***	***3.0E-02***	***1.5E+02***	***5.2E-05***	***1.6E+00***	***7.4E+02***
	SD%		21.51%	17.66%	27.57%	18.97%	17.41%	41.81%	>100%	/

Table S46. Life Cycle Impact Assessment results of synthesis 2, APC scenario.

			AC (mol H^+ eq)	**CC** (kg CO_2 eq)	**ECOTOX** (CTUe)	**PM** (kg PM 2.5)	**MEU** (kg N eq)	**FEU** (kg P eq)	**TEU** (mol N eq)	**HTOX_c** (CTUh)	**HTOX_nc** (CTUh)
S2	**Step 1**	CPK	2.6E-02	8.0E+00	2.9E+02	2.9E-07	4.9E-03	1.8E-03	5.1E-02	1.0E-08	5.4E-08
		Chlorine (gas)	9.8E-04	2.1E-01	2.4E+00	7.6E-09	2.1E-04	1.7E-04	1.9E-03	1.7E-09	2.8E-09

		Electricity	7.7E-11	2.2E-08	6.8E-08	4.6E-16	1.6E-11	4.5E-12	1.5E-10	5.0E-17	1.4E-16
		Heat	1.1E-04	1.2E-01	7.0E-02	5.7E-10	3.4E-05	4.5E-06	3.6E-04	2.2E-11	2.1E-10
		HCl	3.1E-04	6.0E-01	4.5E+00	4.8E-09	1.3E-04	8.7E-05	1.1E-03	1.4E-10	4.9E-10
	Step 2	Dichloroethane	1.6E-04	4.5E-02	2.8E-01	1.2E-09	3.4E-05	1.9E-05	3.2E-04	1.8E-10	5.3E-10
		TBA-OH	1.2E-01	5.1E+01	1.8E+02	1.3E-06	2.4E-02	7.4E-03	2.5E-01	2.7E-08	1.9E-07
		Petroleoum ether	4.9E-05	1.1E-02	4.2E-02	4.5E-10	8.6E-06	1.6E-06	9.3E-05	2.3E-12	1.0E-10
		Heat	2.8E-05	2.9E-02	1.8E-02	1.4E-10	8.7E-06	1.1E-06	9.1E-05	5.6E-12	5.4E-11
		Electricity	8.3E-11	2.4E-08	7.3E-08	4.9E-16	1.7E-11	4.8E-12	1.7E-10	5.3E-17	1.5E-16
		Waste	1.8E-03	3.6E+00	2.7E+01	2.9E-08	7.5E-04	5.2E-04	6.3E-03	8.6E-10	2.9E-09
		CO_2	0.0E+00	3.6E-02	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
		HCl	0.0E+00	0.0E+00	5.1E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
	Total		***1.5E-01***	***6.3E+01***	***5.1E+02***	***1.7E-06***	***3.0E-02***	***9.9E-03***	***3.1E-01***	***4.0E-08***	***2.5E-07***
	SD%		14.90%	14.47%	>100%	46.46%	13.97%	13.93%	>100%	>100%	60.26%
			IR (kg U^{235} eq)	**LU** (Pts)	**ODP** (kg CFC-11 eq)	**POF** (kg NMVOC eq)	**FRD** (MJ)	**MRD** (kg Sb eq)	**WU** (m^3)	**SS** (µp)	
S2	**Step 1**	CPK	3.2E-01	1.8E+01	2.5E-07	2.9E-02	1.5E+02	4.8E-05	1.4E+00	7.6E+02	
		Chlorine (gas)	5.9E-02	9.0E-01	1.2E-08	5.7E-04	3.5E+00	3.0E-06	7.2E-02	2.5E+01	
		Electricity	5.5E-09	2.2E-07	8.5E-17	6.2E-11	3.6E-07	8.1E-14	2.2E-08	1.9E-06	
		Heat	1.8E-03	4.4E-02	4.5E-09	1.9E-04	1.8E+00	1.2E-07	2.6E-03	6.5E-03	
		HCl	4.3E-03	1.6E-01	1.9E-09	3.2E-04	9.0E-01	2.6E-07	1.7E-02	2.4E-02	
	Step 2	Dichloroethane	7.1E-03	1.4E-01	2.2E-09	3.0E-04	1.1E+00	5.4E-07	1.3E-02	5.0E+00	
		TBA-OH	1.1E+00	5.7E+01	1.3E-06	1.1E-01	6.7E+02	1.2E-04	1.0E+01	3.3E+00	
		Petroleoum ether	2.4E-04	4.7E-02	6.7E-10	1.1E-04	5.4E-01	8.4E-08	4.9E-03	1.5E-03	
		Heat	4.6E-04	1.1E-02	1.1E-09	4.9E-05	4.7E-01	3.1E-08	6.5E-04	1.6E-03	
		Electricity	5.9E-09	2.4E-07	9.1E-17	6.6E-11	3.8E-07	8.7E-14	2.3E-08	2.0E-06	
		Waste	2.6E-02	9.8E-01	1.1E-08	1.9E-03	5.4E+00	1.5E-06	1.0E-01	1.4E-01	
		CO_2	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1.0E+00	
		HCl	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1.7E-01	
	Total		***1.6E+00***	***7.7E+01***	***1.5E-06***	***1.5E-01***	***8.3E+02***	***1.8E-04***	***1.2E+01***	***7.9E+02***	
	SD%		17.31%	25.00%	21.73%	18.26%	15.20%	44.81%	>100%	/	

Table S47. Life Cycle Impact Assessment results of synthesis 3, APC scenario.

			AC (mol H^+ eq)	**CC** (kg CO_2 eq)	**ECOTOX** (CTUe)	**PM** (kg PM 2.5)	**MEU** (kg N eq)	**FEU** (kg P eq)	**TEU** (mol N eq)	**HTOX_c** (CTUh)	**HTOX_nc** (CTUh)
S3	**Step 1**	Br-CPK	7.0E-02	2.3E+01	4.9E+02	7.9E-07	1.3E-02	4.3E-03	1.3E-01	2.2E-08	1.3E-07
		NaOH	1.5E-02	2.6E+00	2.0E+01	1.4E-07	3.1E-03	1.3E-03	3.1E-02	1.4E-08	3.7E-08

		Cooling energy	2.1E-04	8.1E-02	1.7E-01	1.5E-09	3.8E-05	1.6E-05	4.1E-04	1.5E-11	7.9E-10
		Electricity	7.8E-11	2.2E-08	6.8E-08	4.6E-16	1.6E-11	4.5E-12	1.6E-10	5.0E-17	1.4E-16
		NaBr	3.2E-03	6.3E+00	4.8E+01	5.1E-08	1.3E-03	9.2E-04	1.1E-02	1.5E-09	5.1E-09
	Step 2	Water	1.4E-07	1.3E-05	1.7E-03	1.1E-12	1.1E-08	5.8E-09	1.1E-07	2.9E-14	1.9E-13
		HCl	1.1E-06	1.9E-04	2.1E-03	7.8E-12	1.8E-07	1.1E-07	1.6E-06	6.9E-13	2.5E-12
		Petroleoum ether	6.2E-04	1.4E-01	5.3E-01	5.8E-09	1.1E-04	2.0E-05	1.2E-03	2.9E-11	1.3E-09
		Electricity	5.8E-12	1.6E-09	5.0E-09	3.4E-17	1.2E-12	3.3E-13	1.2E-11	3.7E-18	1.0E-17
		Wastewater	1.6E-08	3.9E-06	1.5E-05	3.9E-13	4.4E-09	1.3E-09	3.9E-08	1.9E-15	4.3E-14
		CO_2	0.0E+00	5.3E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
	Total		***8.9E-02***	***3.3E+01***	***5.6E+02***	***9.9E-07***	***1.7E-02***	***6.5E-03***	***1.7E-01***	***3.8E-08***	***1.7E-07***
	SD%		13.39%	11.64%	>100%	45.48%	13.75%	14.30%	>100%	>100%	89.76%
			IR (kg U^{235} eq)	**LU** (Pts)	**ODP** (kg CFC-11 eq)	**POF** (kg NMVOC eq)	**FRD** (MJ)	**MRD** (kg Sb eq)	**WU** (m^3)	**SS** (µp)	
S3	**Step 1**	Br-CPK	7.4E-01	3.9E+01	6.5E-07	6.8E-02	3.6E+02	1.0E-04	2.8E+00	1.9E+03	
		NaOH	3.1E-01	8.7E+00	3.5E-07	9.2E-03	3.5E+01	2.5E-05	1.5E+00	2.7E-01	
		Cooling energy	2.8E-03	8.8E-02	1.1E-09	1.9E-04	1.1E+00	8.9E-07	1.7E-02	6.2E+00	
		Electricity	5.5E-09	2.2E-07	8.5E-17	6.2E-11	3.6E-07	8.2E-14	2.2E-08	1.9E-06	
		NaBr	4.5E-02	1.7E+00	2.0E-08	3.3E-03	9.5E+00	2.7E-06	1.8E-01	2.5E-01	
	Step 2	Water	1.7E-06	5.6E-05	5.1E-12	4.3E-08	1.7E-04	1.7E-10	1.5E-03	1.3E-05	
		HCl	4.0E-05	7.2E-04	3.2E-11	5.5E-07	3.3E-03	3.0E-09	9.2E-05	2.2E-05	
		Petroleoum ether	3.1E-03	5.9E-01	8.5E-09	1.4E-03	6.9E+00	1.1E-06	6.2E-02	1.9E-02	
		Electricity	4.1E-10	1.6E-08	6.3E-18	4.6E-12	2.7E-08	6.0E-15	1.6E-09	1.4E-07	
		Wastewater	2.8E-07	2.8E-05	2.6E-14	1.2E-08	3.9E-05	2.9E-11	-1.4E-03	-1.0E-08	
		CO_2	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1.5E+01	
	Total		***1.1E+00***	***5.0E+01***	***1.0E-06***	***8.2E-02***	***4.1E+02***	***1.3E-04***	***4.6E+00***	***1.9E+03***	
	SD%		20.72%	16.42%	24.38%	17.24%	15.11%	38.56%	>100%	/	

Table S48. Life Cycle Impact Assessment results of synthesis 4, APC scenario.

			AC (mol H^+ eq)	**CC** (kg CO_2 eq)	**ECOTOX** (CTUe)	**PM** (kg PM 2.5)	**MEU** (kg N eq)	**FEU** (kg P eq)	**TEU** (mol N eq)	**HTOX_c** (CTUh)	**HTOX_nc** (CTUh)
S4	**Step 1**	CPK	2.4E-02	7.5E+00	2.8E+02	2.7E-07	4.6E-03	1.7E-03	4.7E-02	9.6E-09	5.1E-08
		TBA-Br	1.6E-05	6.5E-03	1.8E-02	1.7E-10	3.0E-06	8.8E-07	3.1E-05	2.7E-12	2.3E-11
		Carbon tetrachloride	1.7E-04	1.9E-02	2.2E-01	2.8E-09	3.3E-05	4.4E-07	3.6E-04	6.4E-12	7.4E-10
		NaOH	2.9E-03	5.2E-01	3.9E+00	2.8E-08	6.0E-04	2.5E-04	6.0E-03	2.7E-09	7.3E-09
		Electricity	9.0E-10	2.6E-07	7.9E-07	5.3E-15	1.9E-10	5.2E-11	1.8E-09	5.8E-16	1.6E-15
		Heat	1.2E-03	1.2E+00	7.3E-01	5.9E-09	3.6E-04	4.7E-05	3.7E-03	2.3E-10	2.2E-09

		Waste	3.3E-04	6.4E-01	4.9E+00	5.2E-09	1.3E-04	9.4E-05	1.1E-03	1.5E-10	5.2E-10
	Step 2	Saturated brine	4.7E-06	6.7E-04	6.4E-03	4.8E-11	1.0E-06	3.7E-07	9.6E-06	3.1E-13	1.5E-11
		Dichloromethane	2.8E-04	3.7E-02	6.0E-01	5.6E-09	5.6E-05	5.5E-07	6.2E-04	5.9E-12	6.8E-10
		Electricity	6.4E-10	1.8E-07	5.6E-07	3.8E-15	1.3E-10	3.7E-11	1.3E-09	4.1E-16	1.2E-15
		Waste	9.4E-06	1.8E-02	1.4E-01	1.5E-10	3.9E-06	2.7E-06	3.2E-05	4.4E-12	1.5E-11
		CO_2	0.0E+00	5.3E-03	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
		HCl	0.0E+00	0.0E+00	1.9E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
	Total		***2.9E-02***	***9.9E+00***	***2.9E+02***	***3.2E-07***	***5.8E-03***	***2.0E-03***	***5.9E-02***	***1.3E-08***	***6.2E-08***
	SD%		17.76%	15.38%	>100%	41.19%	16.85%	17.30%	>100%	>100%	72.35%
			IR (kg U^{235} eq)	**LU** (Pts)	**ODP** (kg CFC-11 eq)	**POF** (kg NMVOC eq)	**FRD** (MJ)	**MRD** (kg Sb eq)	**WU** (m^3)	**SS** (µp)	
S4	**Step 1**	CPK	3.0E-01	1.7E+01	2.3E-07	2.7E-02	1.4E+02	4.4E-05	1.3E+00	7.1E+02	
		TBA-Br	1.3E-04	6.7E-03	1.7E-10	1.4E-05	8.8E-02	1.5E-08	1.3E-03	4.2E-04	
		Carbon tetrachloride	5.0E-06	1.6E-03	2.4E-12	1.0E-04	3.7E-01	3.7E-09	2.7E-02	2.3E+00	
		NaOH	6.0E-02	1.7E+00	6.8E-08	1.8E-03	6.8E+00	4.8E-06	2.9E-01	5.4E-02	
		Electricity	6.4E-08	2.6E-06	9.9E-16	7.2E-10	4.2E-06	9.5E-13	2.5E-07	2.2E-05	
		Heat	1.9E-02	4.5E-01	4.7E-08	2.0E-03	1.9E+01	1.3E-06	2.7E-02	6.8E-02	
		Waste	4.6E-03	1.8E-01	2.0E-09	3.4E-04	9.7E-01	2.7E-07	1.8E-02	2.5E-02	
	Step 2	Saturated brine	6.2E-05	4.3E-03	8.1E-12	2.9E-06	8.3E-03	2.0E-08	6.2E-04	9.0E-05	
		Dichloromethane	5.2E-06	1.4E-03	5.0E-07	1.7E-04	4.0E-01	2.6E-09	4.6E-03	4.1E+00	
		Electricity	4.5E-08	1.8E-06	7.0E-16	5.1E-10	2.9E-06	6.7E-13	1.8E-07	1.6E-05	
		Waste	1.3E-04	5.0E-03	5.7E-11	9.7E-06	2.8E-02	7.8E-09	5.2E-04	7.2E-04	
		CO_2	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1.5E-01	
		HCl	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.3E-02	
	Total		***3.8E-01***	***1.9E+01***	***8.6E-07***	***3.2E-02***	***1.6E+02***	***5.1E-05***	***1.7E+00***	***7.2E+02***	
	SD%		25.08%	15.09%	27.52%	20.98%	18.96%	46.85%	>100%	/	

Table S49. Life Cycle Impact Assessment results of synthesis 5, APC scenario.

			AC (mol H^+ eq)	**CC** (kg CO_2 eq)	**ECOTOX** (CTUe)	**PM** (kg PM 2.5)	**MEU** (kg N eq)	**FEU** (kg P eq)	**TEU** (mol N eq)	**HTOX_c** (CTUh)	**HTOX_nc** (CTUh)
S5	**Step 1**	CPK	2.8E-02	8.6E+00	3.2E+02	3.1E-07	5.3E-03	1.9E-03	5.5E-02	1.1E-08	5.8E-08
		Di-tert-butyl peroxide	7.4E-02	8.2E+00	4.0E+01	5.0E-07	5.6E-03	1.9E-03	5.4E-02	1.6E-09	4.1E-08
		Dichloromethane	8.3E-05	1.1E-02	1.7E-01	1.6E-09	1.6E-05	1.6E-07	1.8E-04	1.7E-12	2.0E-10
		Electricity	5.8E-09	1.6E-06	5.0E-06	3.4E-14	1.2E-09	3.3E-10	1.2E-08	3.7E-15	1.0E-14
		Waste	2.6E-03	5.2E+00	3.9E+01	4.2E-08	1.1E-03	7.6E-04	9.2E-03	1.2E-09	4.2E-09
		CO_2	0.0E+00	1.6E-03	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00

		HCl	0.0E+00	0.0E+00	5.4E+01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
	Step 2	Sodium hydrogen sulfite	1.0E-03	2.7E-02	3.3E-01	6.9E-09	3.1E-05	1.3E-05	3.2E-04	7.0E-11	4.2E-10
		Water	2.1E-10	2.0E-08	2.5E-06	1.7E-15	1.7E-11	8.5E-12	1.6E-10	4.2E-17	2.8E-16
		Electricity	4.6E-11	1.3E-08	4.1E-08	2.7E-16	9.6E-12	2.7E-12	9.3E-11	3.0E-17	8.4E-17
		Wastewater	2.4E-11	5.7E-09	2.2E-08	5.7E-16	6.6E-12	2.0E-12	5.7E-11	2.8E-18	6.3E-17
		Waste	2.1E-05	4.2E-02	3.2E-01	3.4E-10	8.7E-06	6.1E-06	7.4E-05	1.0E-11	3.4E-11
	Step 3	Water	4.6E-08	4.3E-06	5.5E-04	3.7E-13	3.7E-09	1.9E-09	3.6E-08	9.4E-15	6.2E-14
		Heat	2.2E-04	2.3E-01	1.4E-01	1.1E-09	6.7E-05	8.8E-06	7.0E-04	4.3E-11	4.2E-10
		Waste	1.1E-05	2.1E-02	1.6E-01	1.7E-10	4.5E-06	3.1E-06	3.8E-05	5.1E-12	1.7E-11
	Total		***1.1E-01***	***2.2E+01***	***4.5E+02***	***8.7E-07***	***1.2E-02***	***4.6E-03***	***1.2E-01***	***1.4E-08***	***1.0E-07***
	SD%		18.88%	15.70%	>100%	38.14%	16.72%	16.55%	>100%	>100%	65.28%
			IR (kg U^{235} eq)	**LU** (Pts)	**ODP** (kg CFC-11 eq)	**POF** (kg NMVOC eq)	**FRD** (MJ)	**MRD** (kg Sb eq)	**WU** (m^3)	**SS** (µp)	
S5	**Step 1**	CPK	3.4E-01	2.0E+01	2.7E-07	3.1E-02	1.6E+02	5.1E-05	1.5E+00	8.2E+02	
		Di-tert-butyl peroxide	1.0E+00	2.9E+01	1.7E-07	2.2E-02	2.0E+02	4.4E-05	1.2E+01	9.0E+02	
		Dichloromethane	1.5E-06	4.0E-04	1.5E-07	4.9E-05	1.2E-01	7.6E-10	1.4E-03	1.2E+00	
		Electricity	4.1E-07	1.6E-05	6.3E-15	4.6E-09	2.7E-05	6.0E-12	1.6E-06	1.4E-04	
		Heat	3.1E-04	7.4E-03	7.6E-10	3.3E-05	3.1E-01	2.1E-08	4.3E-04	1.1E-03	
		Waste	3.7E-02	1.4E+00	1.6E-08	2.7E-03	7.8E+00	2.2E-06	1.5E-01	2.0E-01	
		CO_2	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	4.3E-02	
		HCl	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1.8E+01	
	Step 2	Sodium hydrogen sulfite	3.0E-03	1.0E-01	1.3E-09	1.5E-04	3.7E-01	6.2E-07	1.0E-02	5.1E-03	
		Water	2.5E-09	8.2E-08	7.5E-15	6.4E-11	2.6E-07	2.6E-13	2.2E-06	1.9E-08	
		Electricity	3.3E-09	1.3E-07	5.1E-17	3.7E-11	2.1E-07	4.9E-14	1.3E-08	1.1E-06	
		Wastewater	4.1E-10	4.2E-08	3.8E-17	1.8E-11	5.7E-08	4.3E-14	-2.1E-06	-1.5E-11	
		Waste	3.0E-04	1.1E-02	1.3E-10	2.2E-05	6.3E-02	1.8E-08	1.2E-03	1.6E-03	
	Step 3	Water	5.4E-07	1.8E-05	1.7E-12	1.4E-08	5.7E-05	5.7E-11	4.8E-04	4.2E-06	
		Heat	3.6E-03	8.6E-02	8.8E-09	3.8E-04	3.6E+00	2.4E-07	5.0E-03	1.3E-02	
		Waste	1.5E-04	5.9E-03	6.7E-11	1.1E-05	3.2E-02	9.1E-09	6.0E-04	8.4E-04	
	Total		***1.4E+00***	***5.0E+01***	***6.1E-07***	***5.7E-02***	***3.7E+02***	***9.8E-05***	***1.3E+01***	***1.7E+03***	
	SD%		18.31%	17.59%	21.17%	17.67%	16.50%	42.63%	>100%	/	

Table S50. Life Cycle Impact Assessment results of synthesis 6, APC scenario.

			AC (mol H^+ eq)	**CC** (kg CO_2 eq)	**ECOTOX** (CTUe)	**PM** (kg PM 2.5)	**MEU** (kg N eq)	**FEU** (kg P eq)	**TEU** (mol N eq)	**HTOX_c** (CTUh)	**HTOX_nc** (CTUh)
S6	**Step 1**	Benzothrichloride	9.5E-03	2.3E+00	1.4E+01	7.7E-08	1.8E-03	9.6E-04	1.7E-02	8.6E-09	2.1E-08
		N,N dimethyl formamide	1.5E-03	3.4E-01	4.0E+00	1.9E-08	2.1E-04	6.3E-05	4.3E-03	6.3E-11	1.9E-09

		Cyclohexanone	1.0E-02	3.0E+00	2.5E+01	1.1E-07	1.8E-03	5.8E-04	1.9E-02	2.3E-09	2.0E-08
		Electricity	9.9E-11	2.8E-08	8.7E-08	5.9E-16	2.1E-11	5.7E-12	2.0E-10	6.4E-17	1.8E-16
		CO_2	0.0E+00	1.8E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
		NO_2	4.7E-02	0.0E+00	0.0E+00	1.0E-07	2.5E-02	0.0E+00	2.7E-01	0.0E+00	0.0E+00
	Step 2	Petroleoum ether	7.7E-05	1.8E-02	6.7E-02	7.2E-10	1.4E-05	2.5E-06	1.5E-04	3.6E-12	1.6E-10
		NaOH	2.8E-03	5.0E-01	3.7E+00	2.7E-08	5.8E-04	2.4E-04	5.7E-03	2.6E-09	7.0E-09
		Water	5.0E-08	4.6E-06	5.9E-04	3.9E-13	4.0E-09	2.0E-09	3.9E-08	1.0E-14	6.7E-14
		Cooling energy	9.8E-03	3.8E+00	7.9E+00	7.2E-08	1.8E-03	7.3E-04	1.9E-02	6.9E-10	3.7E-08
		CO_2	0.0E+00	6.7E-02	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
		Wastewater	5.7E-09	1.4E-06	5.3E-06	1.4E-13	1.5E-09	4.7E-10	1.3E-08	6.7E-16	1.5E-14
		Waste	3.8E-04	7.4E-01	5.6E+00	6.0E-09	1.5E-04	1.1E-04	1.3E-03	1.8E-10	6.0E-10
	Total		***8.2E-02***	***1.1E+01***	***6.0E+01***	***4.1E-07***	***3.1E-02***	***2.7E-03***	***3.4E-01***	***1.5E-08***	***8.7E-08***
	SD%		10.81%	12.91%	>100%	37.67%	11.64%	11.72%	>100%	>100%	92.26%

			IR (kg U^{235} eq)	**LU** (Pts)	**ODP** (kg CFC-11 eq)	**POF** (kg NMVOC eq)	**FRD** (MJ)	**MRD** (kg Sb eq)	**WU** (m^3)	**SS** (µp)
S6	**Step 1**	Benzothrichloride	3.3E-01	7.1E+00	1.4E-07	1.0E-02	6.2E+01	2.0E-05	6.0E-01	2.5E+02
		N,N dimethyl formamide	6.8E-03	7.0E-01	6.8E-09	1.1E-03	6.1E+00	1.8E-06	8.2E-02	3.0E-02
		Cyclohexanone	9.7E-02	7.8E+00	8.1E-08	1.3E-02	6.5E+01	2.1E-05	3.4E-01	2.7E+02
		Electricity	7.0E-09	2.8E-07	1.1E-16	7.9E-11	4.6E-07	1.0E-13	2.8E-08	2.4E-06
		CO_2	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.1E+00
		NO_2	0.0E+00	0.0E+00	0.0E+00	6.4E-02	0.0E+00	0.0E+00	0.0E+00	2.4E-01
	Step 2	Petroleoum ether	3.8E-04	7.4E-02	1.1E-09	1.8E-04	8.6E-01	1.3E-07	7.8E-03	2.4E-03
		NaOH	5.8E-02	1.6E+00	6.5E-08	1.7E-03	6.5E+00	4.6E-06	2.8E-01	5.2E-02
		Water	5.8E-07	1.9E-05	1.8E-12	1.5E-08	6.1E-05	6.1E-11	5.2E-04	4.5E-06
		CO_2	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1.9E+00
		Wastewater	9.8E-08	9.9E-06	9.0E-15	4.3E-09	1.4E-05	1.0E-11	-5.0E-04	-3.6E-09
		Waste	5.3E-03	2.0E-01	2.3E-09	3.9E-04	1.1E+00	3.1E-07	2.1E-02	2.9E-02
	Total		***6.2E-01***	***2.2E+01***	***3.5E-07***	***9.9E-02***	***1.9E+02***	***8.9E-05***	***2.1E+00***	***8.2E+02***
	SD%		19.59%	15.76%	28.95%	11.71%	12.50%	39.96%	>100%	/

Table S51. Life Cycle Impact Assessment results of synthesis 1, SAM scenario.

	AC (mol H^+ eq)	**CC** (kg CO_2 eq)	**ECOTOX** (CTUe)	**PM** (kg PM 2.5)	**MEU** (kg N eq)	**FEU** (kg P eq)	**TEU** (mol N eq)	**HTOX_c** (CTUh)	**HTOX_nc** (CTUh)

S1	**Step 1**	CPK	2.4E-02	7.5E+00	2.7E+02	2.7E-07	4.6E-03	1.7E-03	4.7E-02	9.6E-09	5.1E-08
		Chlorine (gas)	1.1E-03	2.3E-01	2.6E+00	8.3E-09	2.3E-04	1.9E-04	2.0E-03	1.8E-09	3.0E-09
		HCl	1.8E-04	3.5E-01	2.7E+00	2.8E-09	7.4E-05	5.1E-05	6.2E-04	8.5E-11	2.8E-10
	Step 2	NaOH	1.4E-03	2.6E-01	2.0E+00	1.4E-08	3.0E-04	1.2E-04	3.0E-03	1.4E-09	3.7E-09
		TBA-Br	5.4E-06	2.2E-03	6.3E-03	5.8E-11	1.0E-06	3.0E-07	1.1E-05	9.4E-13	7.9E-12
		Heat	9.9E-05	1.0E-01	6.2E-02	5.1E-10	3.1E-05	4.0E-06	3.2E-04	2.0E-11	1.9E-10
		NaCl	2.9E-04	5.7E-01	4.3E+00	4.6E-09	1.2E-04	8.2E-05	1.0E-03	1.4E-10	4.6E-10
	Total		***2.7E-02***	***9.0E+00***	***2.9E+02***	***3.0E-07***	***5.4E-03***	***2.1E-03***	***5.4E-02***	***1.3E-08***	***5.8E-08***
	SD%		14.58%	11.17%	>100%	45.84%	13.55%	12.96%	>100%	>100%	113.86%

			IR (kg U^{235} eq)	**LU** (Pts)	**ODP** (kg CFC-11 eq)	**POF** (kg NMVOC eq)	**FRD** (MJ)	**MRD** (kg Sb eq)	**WU** (m^3)	**SS** (µp)
S1	**Step 1**	CPK	3.0E-01	1.7E+01	2.3E-07	2.7E-02	1.4E+02	4.4E-05	1.3E+00	7.1E+02
		Chlorine (gas)	6.5E-02	9.9E-01	1.3E-08	6.3E-04	3.8E+00	3.3E-06	7.8E-02	2.7E+01
		HCl	2.5E-03	9.6E-02	1.1E-09	1.9E-04	5.3E-01	1.5E-07	9.9E-03	1.4E-02
	Step 2	NaOH	3.0E-02	8.5E-01	3.4E-08	9.0E-04	3.4E+00	2.4E-06	1.5E-01	2.7E-02
		TBA-Br	4.6E-05	2.3E-03	5.8E-11	5.0E-06	3.0E-02	5.1E-09	4.6E-04	1.5E-04
		Heat	1.6E-03	3.9E-02	4.0E-09	1.7E-04	1.7E+00	1.1E-07	2.3E-03	5.8E-03
		NaCl	4.1E-03	1.5E-01	1.8E-09	3.0E-04	8.5E-01	2.4E-07	1.6E-02	2.2E-02
	Total		***4.0E-01***	***1.9E+01***	***2.9E-07***	***2.9E-02***	***1.5E+02***	***5.1E-05***	***1.5E+00***	***7.4E+02***
	SD%		20.00%	15.46%	26.57%	17.54%	14.14%	47.75%	>100%	/

Table S52. Life Cycle Impact Assessment results of synthesis 2, SAM scenario.

			AC (mol H^+ eq)	**CC** (kg CO_2 eq)	**ECOTOX** (CTUe)	**PM** (kg PM 2.5)	**MEU** (kg N eq)	**FEU** (kg P eq)	**TEU** (mol N eq)	**HTOX_c** (CTUh)	**HTOX_nc** (CTUh)
S2	**Step 1**	CPK	2.4E-02	7.5E+00	2.7E+02	2.7E-07	4.6E-03	1.7E-03	4.7E-02	9.6E-09	5.1E-08
		Chlorine (gas)	1.1E-03	2.3E-01	2.6E+00	8.3E-09	2.3E-04	1.9E-04	2.0E-03	1.8E-09	3.0E-09
		Heat	1.2E-05	1.2E-02	7.3E-03	6.0E-11	3.6E-06	4.7E-07	3.8E-05	2.3E-12	2.2E-11
		HCl	1.8E-04	3.5E-01	2.7E+00	2.8E-09	7.4E-05	5.1E-05	6.2E-04	8.4E-11	2.8E-10
	Step 2	Dichloroethane	1.2E-04	3.3E-02	2.1E-01	8.7E-10	2.5E-05	1.4E-05	2.4E-04	1.3E-10	4.0E-10
		TBA-OH	9.7E-02	3.9E+01	1.4E+02	1.0E-06	1.9E-02	5.7E-03	1.9E-01	2.1E-08	1.4E-07
		Petroleoum ether	7.0E-05	1.6E-02	6.0E-02	6.5E-10	1.2E-05	2.2E-06	1.3E-04	3.2E-12	1.4E-10
		Heat	2.8E-04	2.9E-01	1.8E-01	1.5E-09	8.8E-05	1.1E-05	9.2E-04	5.6E-11	5.4E-10
		Waste	2.9E-04	5.6E-01	4.3E+00	4.5E-09	1.2E-04	8.2E-05	9.9E-04	1.4E-10	4.6E-10
		CO_2	0.0E+00	3.2E-02	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
		HCl	0.0E+00	0.0E+00	3.8E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
	Total		***1.2E-01***	***4.8E+01***	***4.3E+02***	***1.3E-06***	***2.4E-02***	***7.7E-03***	***2.4E-01***	***3.2E-08***	***2.0E-07***

	SD%		12.77%	13.05%	>100%	43.42%	13.12%	13.12%	>100%	>100%	154.26%
			IR (kg U^{235} eq)	**LU** (Pts)	**ODP** (kg CFC-11 eq)	**POF** (kg NMVOC eq)	**FRD** (MJ)	**MRD** (kg Sb eq)	**WU** (m^3)	**SS** (µp)	
S2	**Step 1**	CPK	3.0E-01	1.7E+01	2.3E-07	2.7E-02	1.4E+02	4.4E-05	1.3E+00	7.1E+02	
		Chlorine (gas)	6.5E-02	9.8E-01	1.3E-08	6.3E-04	3.8E+00	3.3E-06	7.8E-02	2.7E+01	
		Heat	1.9E-04	4.6E-03	4.7E-10	2.0E-05	1.9E-01	1.3E-08	2.7E-04	6.8E-04	
		HCl	2.5E-03	9.6E-02	1.1E-09	1.9E-04	5.3E-01	1.5E-07	9.9E-03	1.4E-02	
	Step 2	Dichloroethane	5.3E-03	1.1E-01	1.6E-09	2.2E-04	8.0E-01	4.0E-07	9.7E-03	3.7E+00	
		TBA-OH	8.8E-01	4.4E+01	9.8E-07	8.7E-02	5.2E+02	9.6E-05	8.0E+00	2.6E+00	
		Petroleoum ether	3.4E-04	6.7E-02	9.5E-10	1.6E-04	7.7E-01	1.2E-07	7.0E-03	2.1E-03	
		Heat	4.7E-03	1.1E-01	1.2E-08	4.9E-04	4.7E+00	3.2E-07	6.5E-03	1.7E-02	
		Waste	4.1E-03	1.5E-01	1.8E-09	3.0E-04	8.5E-01	2.4E-07	1.6E-02	2.2E-02	
		CO_2	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	8.9E-01	
		HCl	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1.3E-01	
	Total		***1.3E+00***	***6.2E+01***	***1.2E-06***	***1.2E-01***	***6.7E+02***	***1.5E-04***	***9.4E+00***	***7.4E+02***	
	SD%		17.97%	23.75%	22.82%	16.36%	13.31%	38.88%	>100%	/	

Table S53. Life Cycle Impact Assessment results of synthesis 3, SAM scenario.

			AC (mol H^+ eq)	**CC** (kg CO_2 eq)	**ECOTOX** (CTUe)	**PM** (kg PM 2.5)	**MEU** (kg N eq)	**FEU** (kg P eq)	**TEU** (mol N eq)	**HTOX_c** (CTUh)	**HTOX_nc** (CTUh)
S3	**Step 1**	Br-CPK	4.2E-02	1.4E+01	2.9E+02	4.7E-07	7.6E-03	2.5E-03	7.8E-02	1.3E-08	7.5E-08
		NaOH	1.4E-03	2.6E-01	2.0E+00	1.4E-08	3.0E-04	1.2E-04	3.0E-03	1.4E-09	3.7E-09
		Heat	1.7E-04	1.8E-01	1.1E-01	8.9E-10	5.4E-05	7.0E-06	5.6E-04	3.4E-11	3.3E-10
		NaBr	5.1E-04	9.9E-01	7.5E+00	8.0E-09	2.1E-04	1.4E-04	1.8E-03	2.4E-10	8.0E-10
	Step 2	Water	8.5E-06	7.9E-04	1.0E-01	6.7E-11	6.7E-07	3.4E-07	6.6E-06	1.7E-12	1.1E-11
		HCl	6.5E-07	1.1E-04	1.2E-03	4.6E-12	1.1E-07	6.3E-08	9.4E-07	4.1E-13	1.5E-12
		Petroleoum ether	3.7E-04	8.4E-02	3.2E-01	3.4E-09	6.5E-05	1.2E-05	7.0E-04	1.7E-11	7.5E-10
		Cooling energy	2.9E-05	1.1E-02	2.3E-02	2.1E-10	5.2E-06	2.1E-06	5.6E-05	2.0E-12	1.1E-10
		Wastewater	2.5E-07	5.9E-05	2.3E-04	5.9E-12	6.7E-08	2.0E-08	5.8E-07	2.9E-14	6.5E-13
		CO_2	0.0E+00	3.2E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
	Total		***4.4E-02***	***1.6E+01***	***3.0E+02***	***5.0E-07***	***8.2E-03***	***2.8E-03***	***8.4E-02***	***1.5E-08***	***8.1E-08***
	SD%		14.06%	11.04%	>100%	41.11%	13.56%	14.11%	>100%	>100%	174.71%
			IR (kg U^{235} eq)	**LU** (Pts)	**ODP** (kg CFC-11 eq)	**POF** (kg NMVOC eq)	**FRD** (MJ)	**MRD** (kg Sb eq)	**WU** (m^3)	**SS** (µp)	
S3	**Step 1**	Br-CPK	4.4E-01	2.3E+01	3.8E-07	4.0E-02	2.1E+02	5.9E-05	1.7E+00	1.1E+03	

		NaOH	3.0E-02	8.5E-01	3.4E-08	9.0E-04	3.4E+00	2.4E-06	1.5E-01	2.7E-02
		Heat	2.9E-03	6.9E-02	7.1E-09	3.0E-04	2.9E+00	2.0E-07	4.0E-03	1.0E-02
		NaBr	7.1E-03	2.7E-01	3.1E-09	5.2E-04	1.5E+00	4.2E-07	2.8E-02	3.9E-02
	Step 2	Water	9.9E-05	3.3E-03	3.0E-10	2.6E-06	1.0E-02	1.0E-08	8.8E-02	7.7E-04
		HCl	2.3E-05	4.2E-04	1.9E-11	3.2E-07	2.0E-03	1.8E-09	5.5E-05	1.3E-05
		Petroleoum ether	1.8E-03	3.5E-01	5.0E-09	8.6E-04	4.1E+00	6.3E-07	3.7E-02	1.1E-02
		Cooling energy	3.8E-04	1.2E-02	1.6E-10	2.6E-05	1.6E-01	1.2E-07	2.3E-03	8.5E-01
		Wastewater	4.2E-06	4.3E-04	3.9E-13	1.8E-07	5.9E-04	4.4E-10	-2.2E-02	-1.6E-07
		CO_2	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	8.9E+00
	Total		***4.8E-01***	***2.5E+01***	***4.3E-07***	***4.3E-02***	***2.2E+02***	***6.3E-05***	***2.0E+00***	***1.1E+03***
	SD%		20.58%	15.24%	24.54%	16.05%	12.72%	37.02%	>100%	/

Table S54. Life Cycle Impact Assessment results of synthesis 4, SAM scenario.

			AC (mol H^+ eq)	**CC** (kg CO_2 eq)	**ECOTOX** (CTUe)	**PM** (kg PM 2.5)	**MEU** (kg N eq)	**FEU** (kg P eq)	**TEU** (mol N eq)	**HTOX_c** (CTUh)	**HTOX_nc** (CTUh)
S4	**Step 1**	CPK	2.4E-02	7.3E+00	2.7E+02	2.6E-07	4.5E-03	1.6E-03	4.6E-02	9.3E-09	4.9E-08
		TBA-Br	1.5E-05	6.3E-03	1.8E-02	1.6E-10	2.9E-06	8.5E-07	3.0E-05	2.6E-12	2.2E-11
		Carbon tetrachloride	4.4E-03	5.0E-01	5.7E+00	7.2E-08	8.6E-04	1.2E-05	9.4E-03	1.7E-10	1.9E-08
		NaOH	2.3E-03	4.1E-01	3.1E+00	2.2E-08	4.7E-04	2.0E-04	4.7E-03	2.1E-09	5.8E-09
		Heat	5.1E-04	5.3E-01	3.2E-01	2.6E-09	1.6E-04	2.1E-05	1.7E-03	1.0E-10	9.8E-10
		Waste	2.7E-07	5.3E-04	4.0E-03	4.3E-12	1.1E-07	7.7E-08	9.3E-07	1.3E-13	4.3E-13
	Step 2	Saturated brine	4.5E-06	6.5E-04	6.2E-03	4.6E-11	9.7E-07	3.6E-07	9.3E-06	3.0E-13	1.5E-11
		Dichloromethane	2.7E-04	3.6E-02	5.8E-01	5.4E-09	5.5E-05	5.3E-07	6.0E-04	5.7E-12	6.6E-10
		Cooling energy	3.7E-05	1.4E-02	2.9E-02	2.7E-10	6.7E-06	2.7E-06	7.1E-05	2.6E-12	1.4E-10
		Electricity	4.5E-08	1.3E-05	4.0E-05	2.7E-13	9.4E-09	2.6E-09	9.1E-08	2.9E-14	8.2E-14
		Waste	6.9E-04	1.4E+00	1.0E+01	1.1E-08	2.8E-04	2.0E-04	2.4E-03	3.2E-10	1.1E-09
		CO_2	0.0E+00	5.2E-03	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
		HCl	0.0E+00	0.0E+00	1.8E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
	Total		***3.2E-02***	***1.0E+01***	***2.9E+02***	***3.8E-07***	***6.3E-03***	***2.0E-03***	***6.5E-02***	***1.2E-08***	***7.7E-08***
	SD%		14.30%	10.66%	>100%	44.77%	12.89%	13.29%	>100%	>100%	76.34%

			IR (kg U^{235} eq)	**LU** (Pts)	**ODP** (kg CFC-11 eq)	**POF** (kg NMVOC eq)	**FRD** (MJ)	**MRD** (kg Sb eq)	**WU** (m^3)	**SS** (μp)
S4	**Step 1**	CPK	2.9E-01	1.6E+01	2.3E-07	2.6E-02	1.3E+02	4.3E-05	1.2E+00	6.9E+02
		TBA-Br	1.3E-04	6.5E-03	1.6E-10	1.4E-05	8.5E-02	1.4E-08	1.3E-03	4.1E-04
		Carbon tetrachloride	1.3E-04	4.3E-02	6.3E-11	2.7E-03	9.7E+00	9.7E-08	7.2E-01	5.9E+01
		NaOH	4.7E-02	1.3E+00	5.3E-08	1.4E-03	5.4E+00	3.8E-06	2.3E-01	4.2E-02

		Heat	8.5E-03	2.0E-01	2.1E-08	8.9E-04	8.6E+00	5.7E-07	1.2E-02	3.0E-02	
		Waste	3.8E-06	1.4E-04	1.7E-12	2.8E-07	8.0E-04	2.3E-10	1.5E-05	2.1E-05	
	Step 2	Saturated brine	6.0E-05	4.2E-03	7.9E-12	2.8E-06	8.1E-03	2.0E-08	6.0E-04	8.7E-05	
		Dichloromethane	5.1E-06	1.3E-03	4.9E-07	1.6E-04	3.9E-01	2.5E-09	4.5E-03	3.9E+00	
		Cooling energy	4.9E-04	1.5E-02	2.0E-10	3.4E-05	2.0E-01	1.6E-07	3.0E-03	1.1E+00	
		Electricity	3.2E-06	1.3E-04	5.0E-14	3.6E-08	2.1E-04	4.7E-11	1.3E-05	1.1E-03	
		Waste	9.7E-03	3.7E-01	4.2E-09	7.1E-04	2.0E+00	5.8E-07	3.8E-02	5.3E-02	
		CO_2	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1.4E-01	
		HCl	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.1E-02	
	Total		***3.5E-01***	***1.8E+01***	***7.9E-07***	***3.2E-02***	***1.6E+02***	***4.8E-05***	***2.3E+00***	***7.5E+02***	
	SD%		26.53%	13.65%	25.50%	16.94%	13.87%	47.67%	>100%	/	

Table S55. Life Cycle Impact Assessment results of synthesis 5, SAM scenario.

			AC (mol H^+ eq)	**CC** (kg CO_2 eq)	**ECOTOX** (CTUe)	**PM** (kg PM 2.5)	**MEU** (kg N eq)	**FEU** (kg P eq)	**TEU** (mol N eq)	**HTOX_c** (CTUh)	**HTOX_nc** (CTUh)
S5	**Step 1**	CPK	1.4E-02	4.2E+00	1.5E+02	1.5E-07	2.6E-03	9.2E-04	2.6E-02	5.3E-09	2.8E-08
		Di-tert-butyl peroxide	7.5E-02	8.3E+00	4.0E+01	5.0E-07	5.6E-03	1.9E-03	5.4E-02	1.6E-09	4.1E-08
		Dichloromethane	8.3E-05	1.1E-02	1.7E-01	1.6E-09	1.7E-05	1.6E-07	1.8E-04	1.7E-12	2.0E-10
		Cooling energy	3.6E-05	1.4E-02	2.9E-02	2.6E-10	6.6E-06	2.7E-06	7.0E-05	2.5E-12	1.4E-10
		Waste	2.1E-03	4.2E+00	3.2E+01	3.4E-08	8.8E-04	6.1E-04	7.4E-03	1.0E-09	3.4E-09
		CO_2	0.0E+00	1.6E-03	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
		HCl	0.0E+00	0.0E+00	5.4E+01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
	Step 2	Sodium hydrogen sulfite	1.0E-03	2.7E-02	3.3E-01	6.9E-09	3.1E-05	1.3E-05	3.2E-04	7.1E-11	4.2E-10
		Water	2.1E-10	2.0E-08	2.5E-06	1.7E-15	1.7E-11	8.6E-12	1.7E-10	4.3E-17	2.9E-16
		Cooling energy	1.7E-04	6.5E-02	1.3E-01	1.2E-09	3.0E-05	1.2E-05	3.2E-04	1.2E-11	6.3E-10
		Wastewater	2.4E-11	5.8E-09	2.3E-08	5.8E-16	6.6E-12	2.0E-12	5.8E-11	2.9E-18	6.4E-17
		Waste	2.1E-05	4.2E-02	3.2E-01	3.4E-10	8.8E-06	6.1E-06	7.4E-05	1.0E-11	3.4E-11
	Step 3	Water	4.7E-08	4.3E-06	5.5E-04	3.7E-13	3.7E-09	1.9E-09	3.6E-08	9.4E-15	6.3E-14
		Cooling energy	2.2E-06	8.4E-04	1.7E-03	1.6E-11	4.0E-07	1.6E-07	4.2E-06	1.5E-13	8.2E-12
		Heat	1.9E-05	1.9E-02	1.2E-02	9.6E-11	5.8E-06	7.5E-07	6.0E-05	3.7E-12	3.6E-11
		Waste	1.1E-05	2.2E-02	1.6E-01	1.7E-10	4.5E-06	3.1E-06	3.8E-05	5.2E-12	1.7E-11
	Total		***9.2E-02***	***1.7E+01***	***2.8E+02***	***7.0E-07***	***9.2E-03***	***3.5E-03***	***8.9E-02***	***8.0E-09***	***7.4E-08***
	SD%		13.02%	10.52%	>100%	40.23%	9.63%	9.81%	>100%	>100%	100.76%
			IR (kg U^{235} eq)	**LU** (Pts)	**ODP** (kg CFC-11 eq)	**POF** (kg NMVOC eq)	**FRD** (MJ)	**MRD** (kg Sb eq)	**WU** (m^3)	**SS** (µp)	
S5	**Step 1**	CPK	1.6E-01	9.4E+00	1.3E-07	1.5E-02	7.5E+01	2.5E-05	7.2E-01	3.9E+02	

	Di-tert-butyl peroxide	1.0E+00	2.9E+01	1.7E-07	2.3E-02	2.0E+02	4.4E-05	1.2E+01	9.0E+02
	Dichloromethane	1.5E-06	4.0E-04	1.5E-07	4.9E-05	1.2E-01	7.6E-10	1.4E-03	1.2E+00
	Cooling energy	4.8E-04	1.5E-02	2.0E-10	3.3E-05	2.0E-01	1.5E-07	3.0E-03	1.1E+00
	Waste	3.0E-02	1.2E+00	1.3E-08	2.2E-03	6.3E+00	1.8E-06	1.2E-01	1.7E-01
	CO_2	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	4.4E-02
	HCl	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1.8E+01
Step 2	Sodium hydrogen sulfite	3.0E-03	1.0E-01	1.3E-09	1.6E-04	3.7E-01	6.3E-07	1.0E-02	5.1E-03
	Water	2.5E-09	8.3E-08	7.6E-15	6.4E-11	2.6E-07	2.6E-13	2.2E-06	1.9E-08
	Cooling energy	2.2E-03	7.0E-02	9.1E-10	1.5E-04	9.1E-01	7.1E-07	1.4E-02	5.0E+00
	Wastewater	4.2E-10	4.2E-08	3.9E-17	1.8E-11	5.8E-08	4.3E-14	-2.1E-06	-1.5E-11
	Waste	3.0E-04	1.1E-02	1.3E-10	2.2E-05	6.3E-02	1.8E-08	1.2E-03	1.6E-03
Step 3	Water	5.5E-07	1.8E-05	1.7E-12	1.4E-08	5.7E-05	5.7E-11	4.8E-04	4.2E-06
	Cooling energy	2.9E-05	9.2E-04	1.2E-11	2.0E-06	1.2E-02	9.2E-09	1.8E-04	6.5E-02
	Heat	3.1E-04	7.3E-03	7.6E-10	3.2E-05	3.1E-01	2.1E-08	4.3E-04	1.1E-03
	Waste	1.5E-04	5.9E-03	6.7E-11	1.1E-05	3.2E-02	9.1E-09	6.1E-04	8.4E-04
Total		***1.2E+00***	***4.0E+01***	***4.6E-07***	***4.0E-02***	***2.8E+02***	***7.2E-05***	***1.3E+01***	***1.3E+03***
SD%		13.43%	19.67%	11.95%	11.24%	10.63%	41.08%	>100%	/

Table S56. Life Cycle Impact Assessment results of synthesis 6, SAM scenario.

			AC (mol H^+ eq)	CC (kg CO_2 eq)	ECOTOX (CTUe)	PM (kg PM 2.5)	MEU (kg N eq)	FEU (kg P eq)	TEU (mol N eq)	HTOX_c (CTUh)	HTOX_nc (CTUh)
S6	Step 1	Benzothrichloride	2.7E-03	6.6E-01	4.1E+00	2.2E-08	5.2E-04	2.8E-04	4.9E-03	2.5E-09	6.0E-09
		N,N dimethyl formamide	2.3E-03	5.3E-01	6.2E+00	2.9E-08	3.2E-04	9.9E-05	6.7E-03	9.9E-11	2.9E-09
		Cyclohexanone	1.6E-02	4.6E+00	3.9E+01	1.7E-07	2.8E-03	9.1E-04	2.9E-02	3.7E-09	3.1E-08
		CO_2	0.0E+00	2.5E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
		NO_2	6.4E-02	0.0E+00	0.0E+00	1.4E-07	3.4E-02	0.0E+00	3.7E-01	0.0E+00	0.0E+00
	Step 2	Petroleoum ether	1.4E-04	3.2E-02	1.2E-01	1.3E-09	2.5E-05	4.5E-06	2.7E-04	6.6E-12	2.9E-10
		NaOH	5.0E-03	9.1E-01	6.8E+00	4.9E-08	1.1E-03	4.3E-04	1.0E-02	4.8E-09	1.3E-08
		Water	9.1E-08	8.5E-06	1.1E-03	7.2E-13	7.2E-09	3.7E-09	7.1E-08	1.8E-14	1.2E-13
		Cooling energy	5.7E-03	2.2E+00	4.6E+00	4.2E-08	1.0E-03	4.2E-04	1.1E-02	4.0E-10	2.1E-08
		Electricity	4.9E-09	1.4E-06	4.3E-06	2.9E-14	1.0E-09	2.8E-10	9.8E-09	3.1E-15	8.9E-15
		CO_2	0.0E+00	1.2E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
		Wastewater	1.0E-08	2.5E-06	9.6E-06	2.5E-13	2.8E-09	8.5E-10	2.5E-08	1.2E-15	2.7E-14
		Waste	6.9E-04	1.3E+00	1.0E+01	1.1E-08	2.8E-04	2.0E-04	2.4E-03	3.2E-10	1.1E-09
	Total		***9.6E-02***	***1.1E+01***	***7.1E+01***	***4.7E-07***	***4.0E-02***	***2.3E-03***	***4.3E-01***	***1.2E-08***	***7.5E-08***
	SD%		6.81%	12.80%	>100%	48.77%	5.89%	5.88%	>100%	>100%	162.37%

			IR (kg U^{235} eq)	LU (Pts)	ODP (kg CFC-11 eq)	POF (kg NMVOC eq)	FRD (MJ)	MRD (kg Sb eq)	WU (m^3)	SS (µp)
S6	Step 1	Benzothrichloride	9.4E-02	2.0E+00	3.9E-08	2.9E-03	1.8E+01	5.7E-06	1.7E-01	7.2E+01
		N,N dimethyl formamide	1.1E-02	1.1E+00	1.1E-08	1.7E-03	9.6E+00	2.9E-06	1.3E-01	4.7E-02
		Cyclohexanone	1.5E-01	1.2E+01	1.3E-07	2.0E-02	1.0E+02	3.3E-05	5.4E-01	4.2E+02
		CO_2	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.9E+00
		NO_2	0.0E+00	0.0E+00	0.0E+00	8.6E-02	0.0E+00	0.0E+00	0.0E+00	3.2E-01
	Step 2	Petroleoum ether	7.0E-04	1.4E-01	1.9E-09	3.3E-04	1.6E+00	2.4E-07	1.4E-02	4.3E-03
		NaOH	1.1E-01	3.0E+00	1.2E-07	3.1E-03	1.2E+01	8.5E-06	5.1E-01	9.4E-02
		Water	1.1E-06	3.5E-05	3.2E-12	2.7E-08	1.1E-04	1.1E-10	9.4E-04	8.3E-06
		Cooling energy	7.5E-02	2.4E+00	3.1E-08	5.2E-03	3.1E+01	2.4E-05	4.7E-01	1.7E+02
		Electricity	3.5E-07	1.4E-05	5.4E-15	3.9E-09	2.2E-05	5.1E-12	1.4E-06	1.2E-04
		CO_2	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	3.4E+00
		Wastewater	1.8E-07	1.8E-05	1.6E-14	7.8E-09	2.5E-05	1.8E-11	-9.1E-04	-6.5E-09
		Waste	9.7E-03	3.7E-01	4.2E-09	7.1E-04	2.0E+00	5.7E-07	3.8E-02	5.3E-02
	Total		***4.5E-01***	***2.1E+01***	***3.3E-07***	***1.2E-01***	***1.8E+02***	***7.5E-05***	***1.9E+00***	***6.7E+02***
	SD%		20.76%	16.29%	26.79%	8.13%	17.87%	34.62%	>100%	/

Table S57. Montecarlo analysis results (synthesis 1, Lab Scale scenario). 95% interpercentil interval

Damage category	Unit	Mean	Median	SD	CV	2.5%	97.5%	SEM
Acidification	mol H^+ eq	5.05E-02	4.97E-02	4.56E-03	9.02E-02	4.12E-02	6.09E-02	4.56E-04
Climate change	kg CO_2 eq	1.42E+01	1.41E+01	1.17E+00	8.26E-02	1.22E+01	1.74E+01	1.17E-01
Ecotoxicity, freshwater	CTUe	1.63E+02	2.26E+02	3.59E+02	2.20E+00	-6.80E+02	7.67E+02	3.59E+01
Eutrophication, freshwater	kg P eq	3.08E-03	2.76E-03	1.24E-03	4.02E-01	1.61E-03	6.75E-03	1.24E-04
Eutrophication, marine	kg N eq	9.69E-03	9.70E-03	8.89E-04	9.18E-02	8.10E-03	1.18E-02	8.89E-05
Eutrophication, terrestrial	mol N eq	1.01E-01	1.00E-01	9.78E-03	9.72E-02	8.22E-02	1.23E-01	9.78E-04
Human toxicity, cancer	CTUh	-4.86E-07	-3.58E-07	5.96E-06	-1.23E+01	-1.53E-05	1.31E-05	5.96E-07
Human toxicity, non-cancer	CTUh	-6.24E-05	-5.74E-05	7.02E-04	-1.13E+01	-1.81E-03	1.53E-03	7.02E-05
Ionising radiation	kBq U^{235} eq	1.98E+00	1.62E+00	1.28E+00	6.48E-01	9.67E-01	4.96E+00	1.28E-01
Land use	Pt	8.02E+01	7.86E+01	1.26E+01	1.58E-01	6.11E+01	1.08E+02	1.26E+00
Ozone depletion	kg CFC11 eq	2.77E-07	2.72E-07	4.33E-08	1.56E-01	2.05E-07	3.67E-07	4.33E-09
Particulate matter	disease inc.	4.39E-07	4.17E-07	9.37E-08	2.13E-01	3.33E-07	7.60E-07	9.37E-09
Photochemical ozone formation	kg NMVOC eq	4.55E-02	4.54E-02	5.79E-03	1.27E-01	3.58E-02	5.83E-02	5.79E-04
Resource use, fossils	MJ	2.58E+02	2.54E+02	2.56E+01	9.94E-02	2.15E+02	3.18E+02	2.56E+00
Resource use, minerals and metals	kg Sb eq	7.20E-05	6.75E-05	2.20E-05	3.06E-01	4.23E-05	1.46E-04	2.20E-06
Water use	m^3 depriv.	-1.22E+01	1.36E+02	8.13E+02	-6.65E+01	-2.17E+03	1.39E+03	8.13E+01

Table S58. Montecarlo analysis results (synthesis 2, Lab Scale scenario). 95% interpercentil interval

Damage category	Unit	Mean	Median	SD	CV	2.5%	97.5%	SEM
Acidification	mol H^+ eq	1.95E-01	1.92E-01	2.34E-02	1.20E-01	1.57E-01	2.42E-01	2.34E-03
Climate change	kg CO_2 eq	7.25E+01	7.15E+01	6.81E+00	9.38E-02	6.04E+01	8.68E+01	6.81E-01
Ecotoxicity, freshwater	CTUe	7.17E+02	5.97E+02	1.17E+03	1.63E+00	-1.55E+03	2.91E+03	1.17E+02
Eutrophication, freshwater	kg P eq	1.13E-02	9.81E-03	5.28E-03	4.66E-01	5.58E-03	2.85E-02	5.28E-04
Eutrophication, marine	kg N eq	3.84E-02	3.79E-02	3.97E-03	1.04E-01	3.17E-02	4.67E-02	3.97E-04
Eutrophication, terrestrial	mol N eq	3.98E-01	3.94E-01	4.12E-02	1.03E-01	3.28E-01	4.81E-01	4.12E-03
Human toxicity, cancer	CTUh	-6.17E-07	-1.12E-07	8.92E-06	-1.45E+01	-1.82E-05	1.83E-05	8.92E-07
Human toxicity, non-cancer	CTUh	-7.16E-05	-1.14E-06	1.06E-03	-1.48E+01	-2.20E-03	2.15E-03	1.06E-04
Ionising radiation	kBq U^{235} eq	4.37E+00	3.31E+00	4.69E+00	1.07E+00	1.75E+00	1.34E+01	4.69E-01
Land use	Pt	1.71E+02	1.69E+02	2.55E+01	1.49E-01	1.21E+02	2.25E+02	2.55E+00
Ozone depletion	kg CFC11 eq	2.78E-05	2.67E-05	6.22E-06	2.24E-01	1.83E-05	4.15E-05	6.22E-07
Particulate matter	disease inc.	1.94E-06	1.89E-06	3.62E-07	1.86E-01	1.39E-06	2.85E-06	3.62E-08
Photochemical ozone formation	kg NMVOC eq	2.03E-01	2.00E-01	2.75E-02	1.35E-01	1.61E-01	2.79E-01	2.75E-03
Resource use, fossils	MJ	1.10E+03	1.07E+03	1.16E+02	1.06E-01	8.82E+02	1.31E+03	1.16E+01
Resource use, minerals and metals	kg Sb eq	2.49E-04	2.36E-04	7.76E-05	3.12E-01	1.37E-04	4.35E-04	7.76E-06
Water use	m^3 depriv.	3.07E+01	5.95E+01	9.48E+02	3.09E+01	-2.43E+03	1.64E+03	9.48E+01

Table S59. Montecarlo analysis results (synthesis 3, Lab Scale scenario). 95% interpercentil interval

Damage category	Unit	Mean	Median	SD	CV	2.5%	97.5%	SEM
Acidification	mol H^+ eq	1.72E-01	1.71E-01	1.41E-02	8.18E-02	1.48E-01	2.05E-01	1.41E-03
Climate change	kg CO_2 eq	1.00E+02	1.01E+02	6.16E+00	6.14E-02	8.80E+01	1.12E+02	6.16E-01
Ecotoxicity, freshwater	CTUe	2.00E+03	1.94E+03	1.36E+03	6.79E-01	-9.49E+02	4.95E+03	1.36E+02
Eutrophication, freshwater	kg P eq	8.58E-03	7.91E-03	3.80E-03	4.43E-01	4.23E-03	1.73E-02	3.80E-04
Eutrophication, marine	kg N eq	3.04E-02	3.02E-02	2.38E-03	7.83E-02	2.51E-02	3.58E-02	2.38E-04
Eutrophication, terrestrial	mol N eq	3.21E-01	3.19E-01	2.63E-02	8.22E-02	2.65E-01	3.78E-01	2.63E-03
Human toxicity, cancer	CTUh	8.91E-07	1.38E-06	4.10E-06	4.60E+00	-8.94E-06	1.00E-05	4.10E-07
Human toxicity, non-cancer	CTUh	1.06E-04	1.71E-04	4.86E-04	4.58E+00	-1.07E-03	1.15E-03	4.86E-05
Ionising radiation	kBq U^{235} eq	2.16E+00	1.97E+00	1.10E+00	5.09E-01	1.05E+00	5.43E+00	1.10E-01
Land use	Pt	1.49E+02	1.47E+02	1.95E+01	1.31E-01	1.16E+02	1.94E+02	1.95E+00
Ozone depletion	kg CFC11 eq	1.77E-06	1.79E-06	1.83E-07	1.03E-01	1.34E-06	2.10E-06	1.83E-08
Particulate matter	disease inc.	1.71E-06	1.64E-06	3.46E-07	2.02E-01	1.27E-06	2.69E-06	3.46E-08
Photochemical ozone formation	kg NMVOC eq	2.46E-01	2.37E-01	4.15E-02	1.69E-01	1.86E-01	3.51E-01	4.15E-03
Resource use, fossils	MJ	1.19E+03	1.19E+03	1.12E+02	9.45E-02	9.40E+02	1.41E+03	1.12E+01
Resource use, minerals and metals	kg Sb eq	2.40E-04	2.30E-04	8.85E-05	3.69E-01	1.29E-04	4.87E-04	8.85E-06
Water use	m^3 depriv.	1.21E+02	9.98E+01	5.43E+02	4.49E+00	-1.23E+03	1.27E+03	5.43E+01

Table S60. Montecarlo analysis results (synthesis 4, Lab Scale scenario). 95% interpercentil interval

Damage category	Unit	Mean	Median	SD	CV	2.5%	97.5%	SEM
Acidification	mol H^+ eq	8.43E-02	8.38E-02	5.83E-03	6.92E-02	7.32E-02	9.58E-02	5.83E-04
Climate change	kg CO_2 eq	2.07E+01	2.06E+01	1.37E+00	6.64E-02	1.85E+01	2.38E+01	1.37E-01
Ecotoxicity, freshwater	CTUe	2.94E+02	2.61E+02	3.05E+02	1.04E+00	-3.40E+02	1.01E+03	3.05E+01
Eutrophication, freshwater	kg P eq	2.94E-03	2.59E-03	1.20E-03	4.10E-01	1.26E-03	6.33E-03	1.20E-04
Eutrophication, marine	kg N eq	1.68E-02	1.67E-02	1.40E-03	8.36E-02	1.39E-02	2.01E-02	1.40E-04
Eutrophication, terrestrial	mol N eq	1.80E-01	1.80E-01	1.51E-02	8.39E-02	1.49E-01	2.17E-01	1.51E-03
Human toxicity, cancer	CTUh	2.10E-07	6.87E-08	2.44E-06	1.16E+01	-5.08E-06	5.76E-06	2.44E-07
Human toxicity, non-cancer	CTUh	2.11E-05	1.36E-05	2.91E-04	1.38E+01	-6.15E-04	6.85E-04	2.91E-05
Ionising radiation	kBq U^{235} eq	9.45E-01	8.24E-01	4.30E-01	4.55E-01	4.70E-01	2.19E+00	4.30E-02
Land use	Pt	4.49E+01	4.34E+01	6.84E+00	1.52E-01	3.46E+01	6.32E+01	6.84E-01
Ozone depletion	kg CFC11 eq	4.89E-05	4.62E-05	1.02E-05	2.09E-01	3.31E-05	7.25E-05	1.02E-06
Particulate matter	disease inc.	1.23E-06	1.21E-06	1.16E-07	9.42E-02	1.00E-06	1.53E-06	1.16E-08
Photochemical ozone formation	kg NMVOC eq	6.56E-02	6.48E-02	6.06E-03	9.25E-02	5.34E-02	7.99E-02	6.06E-04
Resource use, fossils	MJ	2.85E+02	2.83E+02	2.44E+01	8.54E-02	2.39E+02	3.46E+02	2.44E+00
Resource use, minerals and metals	kg Sb eq	5.96E-05	5.48E-05	2.37E-05	3.97E-01	3.16E-05	1.38E-04	2.37E-06
Water use	m^3 depriv.	2.37E+01	6.41E+01	2.61E+02	1.10E+01	-5.94E+02	5.48E+02	2.61E+01

Table S61. Montecarlo analysis results (synthesis 5, Lab Scale scenario). 95% interpercentil interval

Damage category	Unit	Mean	Median	SD	CV	2.5%	97.5%	SEM
Acidification	mol H^+ eq	2.28E-01	2.25E-01	2.35E-02	1.03E-01	1.93E-01	2.86E-01	2.35E-03
Climate change	kg CO_2 eq	3.33E+01	3.34E+01	2.66E+00	7.98E-02	2.79E+01	3.84E+01	2.66E-01
Ecotoxicity, freshwater	CTUe	3.02E+02	2.48E+02	5.79E+02	1.91E+00	-7.88E+02	1.68E+03	5.79E+01
Eutrophication, freshwater	kg P eq	6.60E-03	6.30E-03	1.78E-03	2.70E-01	3.96E-03	1.08E-02	1.78E-04
Eutrophication, marine	kg N eq	1.93E-02	1.93E-02	1.19E-03	6.17E-02	1.70E-02	2.17E-02	1.19E-04
Eutrophication, terrestrial	mol N eq	1.96E-01	1.95E-01	1.27E-02	6.46E-02	1.75E-01	2.24E-01	1.27E-03
Human toxicity, cancer	CTUh	-3.69E-07	-6.00E-08	2.81E-06	-7.62E+00	-6.38E-06	4.93E-06	2.81E-07
Human toxicity, non-cancer	CTUh	-4.95E-05	-6.44E-06	3.34E-04	-6.74E+00	-7.78E-04	5.67E-04	3.34E-05
Ionising radiation	kBq U^{235} eq	2.40E+00	2.11E+00	1.09E+00	4.55E-01	1.34E+00	5.30E+00	1.09E-01
Land use	Pt	8.65E+01	8.52E+01	1.02E+01	1.18E-01	6.91E+01	1.09E+02	1.02E+00
Ozone depletion	kg CFC11 eq	1.51E-05	1.49E-05	2.80E-06	1.85E-01	9.72E-06	2.20E-05	2.80E-07
Particulate matter	disease inc.	1.78E-06	1.76E-06	1.97E-07	1.10E-01	1.48E-06	2.31E-06	1.97E-08
Photochemical ozone formation	kg NMVOC eq	8.50E-02	8.41E-02	8.49E-03	9.99E-02	7.26E-02	1.06E-01	8.49E-04
Resource use, fossils	MJ	4.68E+02	4.68E+02	3.22E+01	6.88E-02	4.09E+02	5.44E+02	3.22E+00
Resource use, minerals and metals	kg Sb eq	1.62E-04	1.48E-04	5.92E-05	3.65E-01	8.89E-05	3.39E-04	5.92E-06
Water use	m^3 depriv.	7.51E+00	5.85E+00	3.29E+02	4.38E+01	-9.08E+02	6.08E+02	3.29E+01

Table S62. Montecarlo analysis results (synthesis 6, Lab Scale scenario). 95% interpercentil interval

Damage category	Unit	Mean	Median	SD	CV	2.5%	97.5%	SEM
Acidification	mol H^+ eq	9.10E-01	9.06E-01	6.72E-02	7.38E-02	7.83E-01	1.04E+00	6.72E-03
Climate change	kg CO_2 eq	6.55E+01	6.57E+01	3.22E+00	4.91E-02	5.80E+01	7.24E+01	3.22E-01
Ecotoxicity, freshwater	CTUe	4.34E+02	4.52E+02	1.23E+03	2.84E+00	-1.74E+03	2.77E+03	1.23E+02
Eutrophication, freshwater	kg P eq	1.18E-02	1.07E-02	4.90E-03	4.14E-01	5.24E-03	2.61E-02	4.90E-04
Eutrophication, marine	kg N eq	3.90E-01	3.87E-01	3.39E-02	8.70E-02	3.25E-01	4.58E-01	3.39E-03
Eutrophication, terrestrial	mol N eq	4.50E+00	4.47E+00	3.75E-01	8.33E-02	3.78E+00	5.25E+00	3.75E-02
Human toxicity, cancer	CTUh	-7.19E-07	-6.39E-07	6.12E-06	-8.52E+00	-1.47E-05	1.04E-05	6.12E-07
Human toxicity, non-cancer	CTUh	-9.33E-05	-1.16E-04	7.26E-04	-7.78E+00	-1.70E-03	1.23E-03	7.26E-05
Ionising radiation	kBq U^{235} eq	2.93E+00	2.47E+00	1.57E+00	5.37E-01	1.49E+00	8.48E+00	1.57E-01
Land use	Pt	1.78E+02	1.76E+02	2.89E+01	1.62E-01	1.29E+02	2.63E+02	2.89E+00
Ozone depletion	kg CFC11 eq	1.35E-06	1.36E-06	9.60E-08	7.11E-02	1.16E-06	1.54E-06	9.60E-09
Particulate matter	disease inc.	4.35E-06	4.12E-06	1.09E-06	2.51E-01	3.16E-06	6.97E-06	1.09E-07
Photochemical ozone formation	kg NMVOC eq	1.10E+00	1.08E+00	9.06E-02	8.27E-02	9.23E-01	1.27E+00	9.06E-03
Resource use, fossils	MJ	1.05E+03	1.04E+03	8.52E+01	8.11E-02	8.94E+02	1.25E+03	8.52E+00
Resource use, minerals and metals	kg Sb eq	3.13E-04	2.88E-04	1.01E-04	3.22E-01	1.65E-04	5.98E-04	1.01E-05
Water use	m^3 depriv.	6.65E+01	1.71E+02	9.68E+02	1.46E+01	-2.48E+03	1.87E+03	9.68E+01

Table S63. Montecarlo analysis results (synthesis 1, APC scenario). 95% interpercentil interval

Damage category	Unit	Mean	Median	SD	CV	2.5%	97.5%	SEM
Acidification	mol H^+ eq	2.99E-02	2.91E-02	4.92E-03	1.65E-01	2.24E-02	4.17E-02	4.92E-04
Climate change	kg CO_2 eq	8.35E+00	8.17E+00	1.14E+00	1.37E-01	6.32E+00	1.08E+01	1.14E-01
Ecotoxicity, freshwater	CTUe	1.74E+02	1.48E+02	2.87E+02	1.65E+00	-4.06E+02	7.45E+02	2.87E+01
Eutrophication, freshwater	kg P eq	1.85E-03	1.57E-03	1.23E-03	6.66E-01	6.99E-04	5.92E-03	1.23E-04
Eutrophication, marine	kg N eq	5.40E-03	5.33E-03	8.25E-04	1.53E-01	4.17E-03	7.35E-03	8.25E-05
Eutrophication, terrestrial	mol N eq	5.98E-02	5.88E-02	9.27E-03	1.55E-01	4.68E-02	8.20E-02	9.27E-04
Human toxicity, cancer	CTUh	8.58E-09	1.14E-08	9.37E-08	1.09E+01	-1.93E-07	1.87E-07	9.37E-09
Human toxicity, non-cancer	CTUh	-1.36E-06	-5.10E-07	2.11E-05	-1.55E+01	-4.88E-05	3.64E-05	2.11E-06
Ionising radiation	kBq U^{235} eq	4.17E-01	3.07E-01	4.82E-01	1.15E+00	1.11E-01	1.31E+00	4.82E-02
Land use	Pt	1.92E+01	1.86E+01	4.13E+00	2.15E-01	1.28E+01	2.81E+01	4.13E-01
Ozone depletion	kg CFC11 eq	2.65E-07	2.61E-07	4.68E-08	1.77E-01	1.87E-07	3.64E-07	4.68E-09
Particulate matter	disease inc.	3.29E-07	3.09E-07	9.07E-08	2.75E-01	2.16E-07	5.49E-07	9.07E-09
Photochemical ozone formation	kg NMVOC eq	2.91E-02	2.83E-02	5.52E-03	1.90E-01	1.97E-02	4.18E-02	5.52E-04
Resource use, fossils	MJ	1.62E+02	1.59E+02	2.82E+01	1.74E-01	1.16E+02	2.31E+02	2.82E+00
Resource use, minerals and metals	kg Sb eq	5.31E-05	5.02E-05	2.22E-05	4.19E-01	2.38E-05	1.09E-04	2.22E-06
Water use	m^3 depriv.	9.47E+00	2.15E+01	7.20E+01	7.61E+00	-1.56E+02	1.22E+02	7.20E+00

Table S64. Montecarlo analysis results (synthesis 2, APC scenario). 95% interpercentil interval

Damage category	Unit	Mean	Median	SD	CV	2.5%	97.5%	SEM
Acidification	mol H^+ eq	1.45E-01	1.45E-01	2.16E-02	1.49E-01	1.03E-01	1.92E-01	2.16E-03
Climate change	kg CO_2 eq	5.17E+01	5.15E+01	7.48E+00	1.45E-01	3.70E+01	6.75E+01	7.48E-01
Ecotoxicity, freshwater	CTUe	4.43E+02	4.53E+02	9.07E+02	2.04E+00	-1.38E+03	2.52E+03	9.07E+01
Eutrophication, freshwater	kg P eq	7.92E-03	7.42E-03	3.68E-03	4.64E-01	3.15E-03	1.81E-02	3.68E-04
Eutrophication, marine	kg N eq	2.82E-02	2.81E-02	3.94E-03	1.40E-01	2.09E-02	3.67E-02	3.94E-04
Eutrophication, terrestrial	mol N eq	3.00E-01	2.98E-01	4.18E-02	1.39E-01	2.23E-01	3.88E-01	4.18E-03
Human toxicity, cancer	CTUh	5.75E-08	9.55E-08	2.88E-07	5.01E+00	-5.49E-07	5.34E-07	2.88E-08
Human toxicity, non-cancer	CTUh	3.21E-06	7.62E-06	6.70E-05	2.09E+01	-1.24E-04	1.37E-04	6.70E-06
Ionising radiation	kBq U^{235} eq	1.17E+00	1.04E+00	7.05E-01	6.01E-01	4.15E-01	3.10E+00	7.05E-02
Land use	Pt	6.76E+01	6.58E+01	1.17E+01	1.73E-01	4.93E+01	9.33E+01	1.17E+00
Ozone depletion	kg CFC11 eq	2.78E-05	2.63E-05	6.95E-06	2.50E-01	1.70E-05	4.58E-05	6.95E-07
Particulate matter	disease inc.	1.56E-06	1.53E-06	3.39E-07	2.17E-01	1.04E-06	2.58E-06	3.39E-08
Photochemical ozone formation	kg NMVOC eq	1.38E-01	1.35E-01	2.52E-02	1.83E-01	9.67E-02	2.06E-01	2.52E-03
Resource use, fossils	MJ	8.09E+02	8.02E+02	1.23E+02	1.52E-01	5.86E+02	1.09E+03	1.23E+01
Resource use, minerals and metals	kg Sb eq	1.54E-04	1.33E-04	6.90E-05	4.49E-01	6.65E-05	3.69E-04	6.90E-06
Water use	m^3 depriv.	2.32E+01	4.99E+01	2.59E+02	1.12E+01	-4.66E+02	4.56E+02	2.59E+01

Table S65. Montecarlo analysis results (synthesis 3, APC scenario). 95% interpercentil interval

Damage category	Unit	Mean	Median	SD	CV	2.5%	97.5%	SEM
Acidification	mol H^+ eq	9.56E-02	9.65E-02	1.28E-02	1.34E-01	6.89E-02	1.16E-01	1.28E-03
Climate change	kg CO_2 eq	2.87E+01	2.89E+01	3.34E+00	1.16E-01	2.26E+01	3.45E+01	3.34E-01
Ecotoxicity, freshwater	CTUe	1.72E+03	1.84E+03	1.08E+03	6.25E-01	-6.42E+02	3.93E+03	1.08E+02
Eutrophication, freshwater	kg P eq	6.09E-03	5.44E-03	2.77E-03	4.54E-01	2.52E-03	1.46E-02	2.77E-04
Eutrophication, marine	kg N eq	1.68E-02	1.72E-02	2.31E-03	1.37E-01	1.20E-02	2.02E-02	2.31E-04
Eutrophication, terrestrial	mol N eq	1.79E-01	1.83E-01	2.56E-02	1.43E-01	1.26E-01	2.20E-01	2.56E-03
Human toxicity, cancer	CTUh	2.76E-08	4.45E-08	2.69E-07	9.74E+00	-5.33E-07	6.13E-07	2.69E-08
Human toxicity, non-cancer	CTUh	-3.88E-06	-2.81E-06	6.39E-05	-1.65E+01	-1.42E-04	1.21E-04	6.39E-06
Ionising radiation	kBq U^{235} eq	9.47E-01	7.21E-01	8.50E-01	8.97E-01	3.39E-01	4.03E+00	8.50E-02
Land use	Pt	5.26E+01	5.13E+01	1.09E+01	2.08E-01	3.48E+01	7.41E+01	1.09E+00
Ozone depletion	kg CFC11 eq	8.89E-07	8.88E-07	1.46E-07	1.64E-01	6.34E-07	1.25E-06	1.46E-08
Particulate matter	disease inc.	1.05E-06	1.01E-06	2.56E-07	2.43E-01	6.93E-07	1.73E-06	2.56E-08
Photochemical ozone formation	kg NMVOC eq	8.47E-02	8.23E-02	1.46E-02	1.72E-01	5.86E-02	1.15E-01	1.46E-03
Resource use, fossils	MJ	4.40E+02	4.36E+02	6.65E+01	1.51E-01	3.14E+02	5.92E+02	6.65E+00
Resource use, minerals and metals	kg Sb eq	1.32E-04	1.17E-04	5.09E-05	3.87E-01	6.04E-05	2.70E-04	5.09E-06
Water use	m^3 depriv.	2.48E+01	3.38E+01	2.29E+02	9.22E+00	-4.65E+02	5.01E+02	2.29E+01

Table S66. Montecarlo analysis results (synthesis 4, APC scenario). 95% interpercentil interval

Damage category	Unit	Mean	Median	SD	CV	2.5%	97.5%	SEM
Acidification	mol H^+ eq	2.95E-02	2.92E-02	5.24E-03	1.77E-01	2.06E-02	4.29E-02	5.24E-04
Climate change	kg CO_2 eq	8.65E+00	8.50E+00	1.33E+00	1.54E-01	6.33E+00	1.18E+01	1.33E-01
Ecotoxicity, freshwater	CTUe	1.73E+02	1.16E+02	2.64E+02	1.53E+00	-3.14E+02	7.59E+02	2.64E+01
Eutrophication, freshwater	kg P eq	1.60E-03	1.55E-03	6.59E-04	4.11E-01	4.87E-04	3.43E-03	6.59E-05
Eutrophication, marine	kg N eq	5.42E-03	5.33E-03	9.13E-04	1.68E-01	3.93E-03	7.76E-03	9.13E-05
Eutrophication, terrestrial	mol N eq	6.01E-02	5.97E-02	1.04E-02	1.73E-01	4.32E-02	8.74E-02	1.04E-03
Human toxicity, cancer	CTUh	-2.70E-09	-8.51E-09	8.05E-08	-2.98E+01	-1.50E-07	1.64E-07	8.05E-09
Human toxicity, non-cancer	CTUh	-2.29E-06	-4.69E-06	1.97E-05	-8.61E+00	-4.11E-05	3.70E-05	1.97E-06
Ionising radiation	kBq U^{235} eq	2.93E-01	2.16E-01	2.12E-01	7.24E-01	1.03E-01	9.55E-01	2.12E-02
Land use	Pt	1.81E+01	1.75E+01	4.54E+00	2.50E-01	1.13E+01	3.03E+01	4.54E-01
Ozone depletion	kg CFC11 eq	8.02E-07	7.89E-07	1.21E-07	1.50E-01	5.87E-07	1.08E-06	1.21E-08
Particulate matter	disease inc.	3.18E-07	2.97E-07	8.75E-08	2.75E-01	1.96E-07	5.27E-07	8.75E-09
Photochemical ozone formation	kg NMVOC eq	3.05E-02	2.94E-02	6.40E-03	2.10E-01	1.99E-02	4.40E-02	6.40E-04
Resource use, fossils	MJ	1.73E+02	1.67E+02	3.28E+01	1.89E-01	1.14E+02	2.56E+02	3.28E+00
Resource use, minerals and metals	kg Sb eq	4.61E-05	4.16E-05	2.16E-05	4.69E-01	2.03E-05	1.15E-04	2.16E-06
Water use	m^3 depriv.	2.66E+00	2.39E+00	7.45E+01	2.80E+01	-1.54E+02	1.85E+02	7.45E+00

Table S67. Montecarlo analysis results (synthesis 5, APC scenario). 95% interpercentil interval

Damage category	Unit	Mean	Median	SD	CV	2.5%	97.5%	SEM
Acidification	mol H^+ eq	1.07E-01	1.06E-01	2.02E-02	1.89E-01	6.98E-02	1.54E-01	2.02E-03
Climate change	kg CO_2 eq	2.07E+01	2.04E+01	3.25E+00	1.57E-01	1.45E+01	2.82E+01	3.25E-01
Ecotoxicity, freshwater	CTUe	2.86E+02	2.77E+02	2.70E+02	9.44E-01	-3.04E+02	9.63E+02	2.70E+01
Eutrophication, freshwater	kg P eq	4.09E-03	3.71E-03	1.56E-03	3.82E-01	1.98E-03	8.23E-03	1.56E-04
Eutrophication, marine	kg N eq	1.16E-02	1.15E-02	1.94E-03	1.67E-01	7.99E-03	1.64E-02	1.94E-04
Eutrophication, terrestrial	mol N eq	1.19E-01	1.17E-01	1.97E-02	1.66E-01	8.11E-02	1.67E-01	1.97E-03
Human toxicity, cancer	CTUh	1.86E-08	1.36E-08	8.20E-08	4.41E+00	-1.47E-07	1.98E-07	8.20E-09
Human toxicity, non-cancer	CTUh	5.89E-07	-8.22E-07	1.86E-05	3.17E+01	-4.30E-05	4.23E-05	1.86E-06
Ionising radiation	kBq U^{235} eq	1.27E+00	1.04E+00	8.29E-01	6.50E-01	7.10E-01	4.44E+00	8.29E-02
Land use	Pt	4.79E+01	4.76E+01	8.77E+00	1.83E-01	3.06E+01	6.70E+01	8.77E-01
Ozone depletion	kg CFC11 eq	5.39E-07	5.37E-07	9.48E-08	1.76E-01	3.68E-07	7.65E-07	9.48E-09
Particulate matter	disease inc.	8.69E-07	8.42E-07	1.84E-07	2.12E-01	5.69E-07	1.33E-06	1.84E-08
Photochemical ozone formation	kg NMVOC eq	5.50E-02	5.34E-02	9.72E-03	1.77E-01	3.60E-02	7.63E-02	9.72E-04
Resource use, fossils	MJ	3.74E+02	3.69E+02	6.17E+01	1.65E-01	2.64E+02	5.13E+02	6.17E+00
Resource use, minerals and metals	kg Sb eq	9.29E-05	8.76E-05	3.96E-05	4.26E-01	3.67E-05	2.19E-04	3.96E-06
Water use	m^3 depriv.	2.80E+00	1.18E+00	9.19E+01	3.29E+01	-1.76E+02	1.63E+02	9.19E+00

Table S68. Montecarlo analysis results (synthesis 6, APC scenario). 95% interpercentil interval

Damage category	Unit	Mean	Median	SD	CV	2.5%	97.5%	SEM
Acidification	mol H^+ eq	8.02E-02	8.05E-02	8.67E-03	1.08E-01	6.47E-02	1.01E-01	8.67E-04
Climate change	kg CO_2 eq	1.03E+01	1.02E+01	1.33E+00	1.29E-01	7.50E+00	1.29E+01	1.33E-01
Ecotoxicity, freshwater	CTUe	1.25E+02	1.30E+02	3.02E+02	2.42E+00	-5.80E+02	7.20E+02	3.02E+01
Eutrophication, freshwater	kg P eq	2.45E-03	2.27E-03	9.23E-04	3.76E-01	1.17E-03	4.74E-03	9.23E-05
Eutrophication, marine	kg N eq	3.04E-02	3.02E-02	3.54E-03	1.16E-01	2.36E-02	3.83E-02	3.54E-04
Eutrophication, terrestrial	mol N eq	3.31E-01	3.30E-01	3.88E-02	1.17E-01	2.55E-01	4.17E-01	3.88E-03
Human toxicity, cancer	CTUh	2.92E-08	2.19E-08	8.78E-08	3.01E+00	-1.34E-07	2.11E-07	8.78E-09
Human toxicity, non-cancer	CTUh	4.40E-06	3.98E-06	2.12E-05	4.82E+00	-4.42E-05	4.67E-05	2.12E-06
Ionising radiation	kBq U^{235} eq	6.20E-01	4.08E-01	5.72E-01	9.22E-01	1.69E-01	2.57E+00	5.72E-02
Land use	Pt	2.17E+01	2.10E+01	4.25E+00	1.96E-01	1.53E+01	3.45E+01	4.25E-01
Ozone depletion	kg CFC11 eq	3.37E-07	3.34E-07	5.31E-08	1.57E-01	2.38E-07	4.43E-07	5.31E-09
Particulate matter	disease inc.	4.18E-07	3.91E-07	1.21E-07	2.90E-01	2.83E-07	6.87E-07	1.21E-08
Photochemical ozone formation	kg NMVOC eq	9.65E-02	9.57E-02	1.13E-02	1.17E-01	7.68E-02	1.22E-01	1.13E-03
Resource use, fossils	MJ	1.92E+02	1.92E+02	2.40E+01	1.25E-01	1.45E+02	2.46E+02	2.40E+00
Resource use, minerals and metals	kg Sb eq	9.51E-05	8.84E-05	3.80E-05	4.00E-01	4.26E-05	1.98E-04	3.80E-06
Water use	m^3 depriv.	4.96E+00	2.28E+01	1.06E+02	2.14E+01	-2.36E+02	1.87E+02	1.06E+01

Table S69. Montecarlo analysis results (synthesis 1, SAM scenario). 95% interpercentil interval

Damage category	Unit	Mean	Median	SD	CV	2.5%	97.5%	SEM
Acidification	mol H^+ eq	2.77E-02	2.70E-02	4.04E-03	1.46E-01	2.18E-02	3.56E-02	4.04E-04
Climate change	kg CO_2 eq	7.41E+00	7.21E+00	8.28E-01	1.12E-01	6.09E+00	9.34E+00	8.28E-02
Ecotoxicity, freshwater	CTUe	1.65E+02	1.52E+02	2.22E+02	1.34E+00	-2.70E+02	6.85E+02	2.22E+01
Eutrophication, freshwater	kg P eq	1.85E-03	1.65E-03	8.48E-04	4.58E-01	8.05E-04	4.22E-03	8.48E-05
Eutrophication, marine	kg N eq	4.93E-03	4.84E-03	6.68E-04	1.35E-01	3.74E-03	6.52E-03	6.68E-05
Eutrophication, terrestrial	mol N eq	5.50E-02	5.42E-02	7.13E-03	1.30E-01	4.23E-02	7.14E-02	7.13E-04
Human toxicity, cancer	CTUh	7.10E-09	-5.41E-09	6.84E-08	9.63E+00	-1.24E-07	1.32E-07	6.84E-09
Human toxicity, non-cancer	CTUh	-3.76E-07	-2.42E-06	1.53E-05	-4.05E+01	-3.04E-05	3.12E-05	1.53E-06
Ionising radiation	kBq U^{235} eq	3.39E-01	2.51E-01	3.86E-01	1.14E+00	1.00E-01	9.55E-01	3.86E-02
Land use	Pt	1.76E+01	1.70E+01	3.52E+00	2.00E-01	1.29E+01	2.77E+01	3.52E-01
Ozone depletion	kg CFC11 eq	2.27E-07	2.23E-07	3.51E-08	1.55E-01	1.71E-07	3.12E-07	3.51E-09
Particulate matter	disease inc.	2.97E-07	2.77E-07	7.89E-08	2.65E-01	2.10E-07	5.38E-07	7.89E-09
Photochemical ozone formation	kg NMVOC eq	2.80E-02	2.73E-02	4.91E-03	1.75E-01	1.93E-02	4.06E-02	4.91E-04
Resource use, fossils	MJ	1.52E+02	1.49E+02	2.15E+01	1.42E-01	1.21E+02	2.03E+02	2.15E+00
Resource use, minerals and metals	kg Sb eq	4.88E-05	4.29E-05	2.33E-05	4.77E-01	1.87E-05	1.04E-04	2.33E-06
Water use	m^3 depriv.	8.11E+00	1.83E+01	6.34E+01	7.82E+00	-1.88E+02	1.23E+02	6.34E+00

Table S70. Montecarlo analysis results (synthesis 2, SAM scenario). 95% interpercentil interval

Damage category	Unit	Mean	Median	SD	CV	2.5%	97.5%	SEM
Acidification	mol H^+ eq	1.12E-01	1.12E-01	1.43E-02	1.28E-01	8.47E-02	1.46E-01	1.43E-03
Climate change	kg CO_2 eq	3.83E+01	3.78E+01	5.00E+00	1.30E-01	2.90E+01	4.99E+01	5.00E-01
Ecotoxicity, freshwater	CTUe	2.33E+02	2.55E+02	7.57E+02	3.25E+00	-1.37E+03	1.66E+03	7.57E+01
Eutrophication, freshwater	kg P eq	5.55E-03	5.00E-03	2.41E-03	4.34E-01	2.11E-03	1.24E-02	2.41E-04
Eutrophication, marine	kg N eq	2.18E-02	2.15E-02	2.86E-03	1.31E-01	1.66E-02	2.91E-02	2.86E-04
Eutrophication, terrestrial	mol N eq	2.34E-01	2.32E-01	3.07E-02	1.31E-01	1.78E-01	3.12E-01	3.07E-03
Human toxicity, cancer	CTUh	5.40E-09	-3.71E-09	2.29E-07	4.24E+01	-4.85E-07	4.08E-07	2.29E-08
Human toxicity, non-cancer	CTUh	-3.76E-06	-3.90E-06	5.71E-05	-1.52E+01	-1.30E-04	9.72E-05	5.71E-06
Ionising radiation	kBq U^{235} eq	1.29E+00	7.79E-01	1.99E+00	1.54E+00	3.39E-01	8.27E+00	1.99E-01
Land use	Pt	5.41E+01	5.32E+01	9.72E+00	1.80E-01	3.80E+01	7.29E+01	9.72E-01
Ozone depletion	kg CFC11 eq	2.08E-05	2.00E-05	4.94E-06	2.37E-01	1.31E-05	3.42E-05	4.94E-07
Particulate matter	disease inc.	1.24E-06	1.16E-06	2.83E-07	2.27E-01	8.73E-07	2.19E-06	2.83E-08
Photochemical ozone formation	kg NMVOC eq	1.07E-01	1.05E-01	1.75E-02	1.64E-01	7.82E-02	1.51E-01	1.75E-03
Resource use, fossils	MJ	6.47E+02	6.35E+02	8.61E+01	1.33E-01	4.87E+02	8.46E+02	8.61E+00
Resource use, minerals and metals	kg Sb eq	1.25E-04	1.12E-04	4.86E-05	3.90E-01	5.61E-05	2.78E-04	4.86E-06
Water use	m^3 depriv.	-2.75E+00	-3.11E+00	2.26E+02	-8.23E+01	-4.60E+02	4.24E+02	2.26E+01

Table S71. Montecarlo analysis results (synthesis 3, SAM scenario). 95% interpercentil interval

Damage category	Unit	Mean	Median	SD	CV	2.5%	97.5%	SEM
Acidification	mol H^+ eq	4.95E-02	4.85E-02	6.96E-03	1.41E-01	3.70E-02	6.44E-02	6.96E-04
Climate change	kg CO_2 eq	1.34E+01	1.35E+01	1.48E+00	1.10E-01	1.05E+01	1.60E+01	1.48E-01
Ecotoxicity, freshwater	CTUe	1.04E+03	9.79E+02	5.34E+02	5.16E-01	1.66E+02	2.29E+03	5.34E+01
Eutrophication, freshwater	kg P eq	2.70E-03	2.50E-03	1.11E-03	4.10E-01	1.16E-03	5.93E-03	1.11E-04
Eutrophication, marine	kg N eq	8.04E-03	8.02E-03	1.09E-03	1.36E-01	6.19E-03	1.03E-02	1.09E-04
Eutrophication, terrestrial	mol N eq	8.79E-02	8.72E-02	1.24E-02	1.41E-01	6.65E-02	1.17E-01	1.24E-03
Human toxicity, cancer	CTUh	1.63E-08	1.35E-08	1.02E-07	6.27E+00	-2.01E-07	2.00E-07	1.02E-08
Human toxicity, non-cancer	CTUh	6.32E-07	1.08E-06	2.53E-05	4.01E+01	-5.44E-05	4.67E-05	2.53E-06
Ionising radiation	kBq U^{235} eq	5.26E-01	3.02E-01	9.19E-01	1.75E+00	1.31E-01	2.54E+00	9.19E-02
Land use	Pt	2.58E+01	2.52E+01	5.31E+00	2.06E-01	1.75E+01	3.95E+01	5.31E-01
Ozone depletion	kg CFC11 eq	3.68E-07	3.71E-07	5.61E-08	1.53E-01	2.63E-07	5.02E-07	5.61E-09
Particulate matter	disease inc.	5.38E-07	5.04E-07	1.32E-07	2.46E-01	3.67E-07	9.03E-07	1.32E-08
Photochemical ozone formation	kg NMVOC eq	4.61E-02	4.49E-02	7.40E-03	1.60E-01	3.42E-02	6.22E-02	7.40E-04
Resource use, fossils	MJ	2.43E+02	2.40E+02	3.09E+01	1.27E-01	1.83E+02	3.00E+02	3.09E+00
Resource use, minerals and metals	kg Sb eq	6.24E-05	5.68E-05	2.31E-05	3.70E-01	2.66E-05	1.18E-04	2.31E-06
Water use	m^3 depriv.	1.99E+01	2.64E+01	9.09E+01	4.56E+00	-2.14E+02	2.10E+02	9.09E+00

Table S71. Montecarlo analysis results (synthesis 4, SAM scenario). 95% interpercentil interval

Damage category	Unit	Mean	Median	SD	CV	2.5%	97.5%	SEM
Acidification	mol H^+ eq	3.21E-02	3.17E-02	4.59E-03	1.43E-01	2.53E-02	4.42E-02	4.59E-04
Climate change	kg CO_2 eq	8.81E+00	8.73E+00	9.39E-01	1.07E-01	7.28E+00	1.13E+01	9.39E-02
Ecotoxicity, freshwater	CTUe	1.60E+02	1.38E+02	2.47E+02	1.55E+00	-4.33E+02	7.50E+02	2.47E+01
Eutrophication, freshwater	kg P eq	1.72E-03	1.55E-03	7.70E-04	4.49E-01	7.10E-04	3.78E-03	7.70E-05
Eutrophication, marine	kg N eq	5.95E-03	5.92E-03	7.67E-04	1.29E-01	4.87E-03	7.68E-03	7.67E-05
Eutrophication, terrestrial	mol N eq	6.57E-02	6.49E-02	8.73E-03	1.33E-01	5.30E-02	8.74E-02	8.73E-04
Human toxicity, cancer	CTUh	7.40E-09	1.44E-08	8.14E-08	1.10E+01	-1.74E-07	1.92E-07	8.14E-09
Human toxicity, non-cancer	CTUh	-1.81E-06	-2.67E-06	1.84E-05	-1.02E+01	-4.65E-05	3.75E-05	1.84E-06
Ionising radiation	kBq U^{235} eq	3.55E-01	2.55E-01	2.71E-01	7.64E-01	1.08E-01	1.18E+00	2.71E-02
Land use	Pt	1.76E+01	1.69E+01	4.67E+00	2.66E-01	1.16E+01	2.92E+01	4.67E-01
Ozone depletion	kg CFC11 eq	7.26E-07	7.12E-07	9.91E-08	1.37E-01	5.46E-07	9.74E-07	9.91E-09
Particulate matter	disease inc.	3.89E-07	3.71E-07	9.92E-08	2.55E-01	2.63E-07	6.61E-07	9.92E-09
Photochemical ozone formation	kg NMVOC eq	3.07E-02	3.00E-02	5.20E-03	1.69E-01	2.20E-02	4.46E-02	5.20E-04
Resource use, fossils	MJ	1.63E+02	1.59E+02	2.26E+01	1.39E-01	1.27E+02	2.23E+02	2.26E+00
Resource use, minerals and metals	kg Sb eq	4.51E-05	4.25E-05	2.15E-05	4.77E-01	1.69E-05	1.18E-04	2.15E-06
Water use	m^3 depriv.	-2.16E+00	2.88E+00	6.63E+01	-3.07E+01	-1.36E+02	1.08E+02	6.63E+00

Table S72. Montecarlo analysis results (synthesis 5, SAM scenario). 95% interpercentil interval

Damage category	Unit	Mean	Median	SD	CV	2.5%	97.5%	SEM
Acidification	mol H^+ eq	9.91E-02	9.65E-02	1.29E-02	1.30E-01	7.56E-02	1.28E-01	1.29E-03
Climate change	kg CO_2 eq	1.74E+01	1.73E+01	1.83E+00	1.06E-01	1.34E+01	2.13E+01	1.83E-01
Ecotoxicity, freshwater	CTUe	1.93E+02	2.02E+02	1.63E+02	8.48E-01	-1.43E+02	5.45E+02	1.63E+01
Eutrophication, freshwater	kg P eq	3.53E-03	3.12E-03	1.42E-03	4.03E-01	1.85E-03	7.66E-03	1.42E-04
Eutrophication, marine	kg N eq	1.07E-02	1.07E-02	1.03E-03	9.66E-02	8.55E-03	1.28E-02	1.03E-04
Eutrophication, terrestrial	mol N eq	1.07E-01	1.08E-01	1.05E-02	9.79E-02	8.52E-02	1.29E-01	1.05E-03
Human toxicity, cancer	CTUh	9.58E-09	7.40E-09	4.59E-08	4.80E+00	-8.50E-08	1.19E-07	4.59E-09
Human toxicity, non-cancer	CTUh	4.22E-07	-1.71E-07	1.18E-05	2.79E+01	-2.27E-05	2.57E-05	1.18E-06
Ionising radiation	kBq U^{235} eq	1.32E+00	1.01E+00	1.33E+00	1.01E+00	7.24E-01	6.54E+00	1.33E-01
Land use	Pt	3.88E+01	3.89E+01	5.21E+00	1.34E-01	2.73E+01	5.15E+01	5.21E-01
Ozone depletion	kg CFC11 eq	1.50E-05	1.49E-05	2.95E-06	1.96E-01	9.62E-06	2.16E-05	2.95E-07
Particulate matter	disease inc.	8.62E-07	8.64E-07	1.03E-07	1.19E-01	6.74E-07	1.09E-06	1.03E-08
Photochemical ozone formation	kg NMVOC eq	4.43E-02	4.49E-02	4.98E-03	1.12E-01	3.26E-02	5.40E-02	4.98E-04
Resource use, fossils	MJ	3.02E+02	2.99E+02	3.21E+01	1.06E-01	2.37E+02	3.72E+02	3.21E+00
Resource use, minerals and metals	kg Sb eq	6.67E-05	6.23E-05	2.74E-05	4.11E-01	3.10E-05	1.53E-04	2.74E-06
Water use	m^3 depriv.	1.80E+01	1.90E+01	6.63E+01	3.68E+00	-1.44E+02	1.49E+02	6.63E+00

Table S73. Montecarlo analysis results (synthesis 6, SAM scenario). 95% interpercentil interval

Damage category	Unit	Mean	Median	SD	CV	2.5%	97.5%	SEM
Acidification	mol H^+ eq	9.74E-02	9.72E-02	6.63E-03	6.81E-02	8.46E-02	1.12E-01	6.63E-04
Climate change	kg CO_2 eq	1.07E+01	1.05E+01	1.37E+00	1.28E-01	8.23E+00	1.46E+01	1.37E-01
Ecotoxicity, freshwater	CTUe	8.96E+01	5.66E+01	2.76E+02	3.07E+00	-4.00E+02	6.14E+02	2.76E+01
Eutrophication, freshwater	kg P eq	2.44E-03	2.10E-03	1.19E-03	4.87E-01	7.77E-04	5.40E-03	1.19E-04
Eutrophication, marine	kg N eq	4.01E-02	4.01E-02	2.36E-03	5.88E-02	3.61E-02	4.55E-02	2.36E-04
Eutrophication, terrestrial	mol N eq	4.39E-01	4.39E-01	2.58E-02	5.88E-02	3.94E-01	4.99E-01	2.58E-03
Human toxicity, cancer	CTUh	1.06E-08	1.55E-08	8.74E-08	8.22E+00	-1.69E-07	1.77E-07	8.74E-09
Human toxicity, non-cancer	CTUh	5.54E-07	8.94E-07	2.04E-05	3.68E+01	-3.73E-05	3.83E-05	2.04E-06
Ionising radiation	kBq U^{235} eq	4.81E-01	2.96E-01	7.81E-01	1.62E+00	1.43E-01	3.56E+00	7.81E-02
Land use	Pt	2.11E+01	2.03E+01	4.38E+00	2.07E-01	1.53E+01	3.16E+01	4.38E-01
Ozone depletion	kg CFC11 eq	3.37E-07	3.32E-07	5.49E-08	1.63E-01	2.58E-07	4.91E-07	5.49E-09
Particulate matter	disease inc.	4.74E-07	4.38E-07	1.27E-07	2.69E-01	3.41E-07	8.90E-07	1.27E-08
Photochemical ozone formation	kg NMVOC eq	1.22E-01	1.20E-01	9.92E-03	8.15E-02	1.04E-01	1.43E-01	9.92E-04
Resource use, fossils	MJ	1.78E+02	1.75E+02	3.18E+01	1.79E-01	1.26E+02	2.69E+02	3.18E+00
Resource use, minerals and metals	kg Sb eq	7.25E-05	6.57E-05	2.51E-05	3.46E-01	4.22E-05	1.28E-04	2.51E-06
Water use	m^3 depriv.	6.54E+00	1.44E+01	1.04E+02	1.59E+01	-2.44E+02	2.03E+02	1.04E+01

Bibliography

1 Q. Wang Yongfei Liu, 2020. CN102267887A
2 H. Shicao, W. Ji, J. Lei, A. Wenliang, M. Guihong and Z. Qi, 2018. CN109503343B
3 E. Meneguzzo, G. Norcini and G. Li Bassi, 2009. WO2009135895A1
4 Q. Chen and Q. Huang, 2018. CN108911959A
5 F. Wang, 2019. CN109694310A
6 J. Sun, 2017. CN109896942A
7 G. J. Minkoff, Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences, 1954, 224, 176–191.
8 TOSOH F TECH, 2015. JP5647782
9 Elservier, Reaxys, https://www.reaxys.com/, (accessed 24 March 2026).
10 L. Xia, Y. Pan, T. Zhao, X. Sun, S. Tao, Y. Chen and S. Xiang, Chin. J. Chem. Eng., 2023, 57, 30–38.
11 M. A. V Ribeiro Da Silva, M. Agostinha, R. Matos, M. S. Miranda, M. Helena, F. A. Sousa, R. M. Borges, D. Santos, M. M. Bizarro and J. A. M. Simões, Struct. Chem.
12 U.S. Department of Commerce, NIST Chemistry WebBook, https://webbook.nist.gov/, (accessed 12 June 2026).
13 The Engineering toolbox, Table of heat capacities of various liquids, https://www.engineeringtoolbox.com/specific-heat-fluids-d_151.html, (accessed 17 November 2025).
14 B. P. Weidema and M. S. Wesnæs, J. Clean. Prod., 1996, 4, 167–174.