SUPPORTING INFORMATION

The environmental performance of producing formate from electrochemical reduction of CO_2 in ionic liquid

Table S1 – Materials quantity and electricity required to produce 1 kg of ionic liquid [P66616][124Triz], as reported in Hollingsworth et al. (2015a, 2015b).

Ionic Liquid [P66614][124Triz]	Quantity for 1 kg of IL	Unit
1,2,4 Triazole	1.25E-01	kg
[P66614][OH]	9.05E-01	kg
Electricity	1.16E+00	MJ

Table S2 – Emissions from mono-ethanolamine (MEA) during the carbon dioxide capture process from flue gas, from Singh et al. (2011).

Emissions from mono-ethanolamine (MEA) usage	Quantity for 1 kg of CO_2	Unit
MEA	6.30E-05	kg
Ammonia	3.50E-05	kg
Formaldehyde	2.62E-04	kg
Acetaldehyde	1.67E-04	kg

Table S3 - Quantity of material required to build the carbon capture unit per ton of CO_2 captured over the lifetime of the unit (30 years). Data from Koornneef et al. (2008).

Carbon capture unit	Quantity for 1 t of CO_2 over the lifetime of the unit	Unit
Steel (high alloyed)	3.37E-06	kg
Concrete	1.06E-08	m^3

Table S4 – Carbon capture removal performances, from Rao and Rubin (2002).

Carbon capture unit removal performances	Efficiency of removal (%)
Carbon dioxide – CO2	90%
Sulfur dioxide – SO2	90%
Nitrogen dioxide – NO2	25%
Ammonia – NH3	0.02%
Hydrogen chloride – HCl	95%
Hydrogen fluoride -HF	90%
Particulate matter – PM	50%

Table S6 – Environmental impacts of 1kg of formate produced via electrochemical reduction, for the baseline scenario: electricity mix in 2020, recycling rate of 99.9%, purification electricity

Impact categories	**TOTAL**	**Carbon Capture**	**Formate production**											
			Total	IL production	Electrochemical reduction							Purification		
					Total	Acetonitrile	Electricity Stirring	Electricity. Applied potential	Platinum Electrode	Silver Electrode	Water	Total	Thermal energy, natural gas	Hazardous wastes
Acidification midpoint [Mole of H+ eq.]	**2.72E-02**	0	2.72E-02	4.81E-04	2.38E-02	1.09E-03	1.69E-02	1.76E-05	5.74E-03	3.70E-05	1.53E-05	2.83E-03	1.97E-03	8.63E-04
Climate change midpoint [kg CO2 eq.]	**8.19E+00**	0	8.19E+00	8.24E-02	5.62E+00	1.37E-01	5.19E+00	5.38E-03	2.86E-01	3.28E-04	4.60E-03	2.49E+00	2.19E+00	3.02E-01
Ecotoxicity freshwater midpoint (v1.09) [CTUe]	**5.25E+00**	0	5.25E+00	2.86E+00	7.78E-01	5.79E-01	1.71E-01	1.77E-04	2.55E-02	6.66E-04	1.22E-03	1.62E+00	4.65E-03	1.61E+00
Eutrophication freshwater [kg P eq.]	**1.87E-04**	0	1.87E-04	6.77E-05	1.61E-05	1.26E-05	3.24E-06	3.36E-09	3.64E-08	1.90E-10	2.17E-07	1.03E-04	4.21E-08	1.03E-04
Eutrophication marine [kg N eq.]	**5.96E-03**	0	5.96E-03	1.40E-04	4.98E-03	5.67E-04	3.95E-03	4.10E-06	4.53E-04	3.18E-07	5.68E-06	8.38E-04	7.19E-04	1.19E-04
Eutrophication terrestrial [Mole of N eq.]	**6.03E-02**	0	6.03E-02	8.20E-04	5.04E-02	2.87E-03	4.25E-02	4.41E-05	4.95E-03	3.43E-06	4.61E-05	9.10E-03	7.95E-03	1.14E-03
Human toxicity midpoint, cancer effects [CTUh]	**5.58E-08**	0	5.58E-08	4.21E-09	7.68E-09	3.05E-09	4.33E-09	4.49E-12	2.52E-10	4.88E-12	3.25E-11	4.39E-08	2.83E-10	4.36E-08
Human toxicity midpoint, non-cancer effects [CTUh]	**3.19E-07**	0	3.19E-07	1.54E-08	2.60E-07	1.61E-08	2.35E-07	2.43E-10	8.18E-09	6.71E-10	3.04E-10	4.38E-08	1.49E-09	4.23E-08
Ionizing radiation midpoint, human health [kBq U235 eq.]	**1.38E+00**	0	1.38E+00	1.19E-02	1.36E+00	5.19E-03	1.35E+00	1.40E-03	3.91E-03	1.66E-06	1.23E-03	1.17E-02	2.83E-03	8.88E-03
Ozone depletion [kg CFC-11 eq.]	**3.72E-08**	0	3.72E-08	8.83E-09	7.40E-09	7.40E-09	2.18E-13	2.26E-16	8.86E-16	2.07E-18	1.91E-16	2.10E-08	5.04E-16	2.10E-08
Particulate matter/Respiratory inorganics [kg PM2.5 eq.]	**1.43E-03**	0	1.43E-03	4.93E-05	1.19E-03	6.27E-05	7.38E-04	7.65E-07	3.86E-04	1.74E-06	7.78E-07	1.86E-04	1.02E-04	8.42E-05
Photochemical ozone formation, human health [kg NMVOC eq.]	**1.59E-02**	0	1.59E-02	2.87E-04	1.29E-02	3.43E-04	1.11E-02	1.15E-05	1.49E-03	3.09E-06	1.10E-05	2.66E-03	2.06E-03	5.98E-04
Resource depletion water [m^3 eq.]	**2.67E-02**	0	2.67E-02	1.06E-03	2.42E-02	1.06E-03	2.04E-02	2.12E-05	1.98E-03	2.64E-06	7.64E-04	1.41E-03	5.92E-04	8.19E-04
Resource depletion, mineral, fossils and renewables, [kg Sb eq.]	**7.68E-05**	0	7.68E-05	2.58E-06	7.14E-05	3.79E-06	1.49E-05	1.55E-08	5.18E-05	8.63E-07	2.54E-09	2.77E-06	4.25E-07	2.34E-06

requirement of 35 MJ/kg and carbon dioxide with a nil market value.

Table S7 – Environmental impacts of 1 kg of formate produced via electrochemical reduction for different recycling rates (RT). The other parameters are: current electricity mix (2020), purification electricity requirement of 35 MJ/kg of output and carbon dioxide with a nil market value.

Impact categories	RT 95%	RT 99%	RT 99.5%	RT 99.9%
Acidification [mol H^+ eq.]	2.71E-01	7.20E-02	4.71E-02	2.72E-02
Climate change [kg CO_2 eq.]	5.08E+01	1.60E+01	1.17E+01	8.19E+00
Ecotoxicity freshwater [CTUe]	4.25E+02	8.24E+01	3.95E+01	5.25E+00
Eutrophication freshwater [kg P eq.]	1.31E-02	2.57E-03	1.24E-03	1.87E-04
Eutrophication marine [kg N eq.]	1.07E-01	2.46E-02	1.42E-02	5.96E-03
Eutrophication terrestrial [mol N eq.]	6.09E-01	1.61E-01	1.05E-01	6.03E-02
Human toxicity, cancer effect [CTUh]	3.02E-06	6.00E-07	2.98E-07	5.58E-08
Human toxicity, non-cancer effects [CTUh]	6.13E-06	1.39E-06	7.94E-07	3.19E-07
Ionising radiation [kg U235 eq.]	3.64E+00	1.80E+00	1.57E+00	1.38E+00
Ozone depletion [CFC-11]	2.94E-06	5.71E-07	2.74E-07	3.72E-08
Particulate matter [kg $PM_{2.5}$ eq.]	1.91E-02	4.68E-03	2.87E-03	1.43E-03
Photochemical ozone formation [kg NMVOC]	1.21E-01	3.52E-02	2.45E-02	1.59E-02
Resource depletion - mineral fossil and renewable [kg Sb eq.]	3.16E-01	7.99E-02	5.03E-02	2.67E-02
Resource deletion – water [m^3 water]	9.76E-04	2.42E-04	1.50E-04	7.68E-05

Table S8 – Environmental impacts of 1 kg formate produced via electrochemical reduction for different thermal energy requirements for the purification step. The other parameters are: current electricity mix (2020), recycling rate at 99.9% and carbon dioxide with a nil market value.

Impact categories	Thermal energy 150 MJ	Thermal energy 35 MJ	Thermal energy 0.483 MJ
Acidification [mol H^+ eq.]	3.36E-02	2.72E-02	2.52E-02
Climate change [kg CO_2 eq.]	1.54E+01	8.19E+00	6.03E+00
Ecotoxicity freshwater [CTUe]	5.27E+00	5.25E+00	5.25E+00
Eutrophication freshwater [kg P eq.]	1.87E-04	1.87E-04	1.87E-04
Eutrophication marine [kg N eq.]	8.32E-03	5.96E-03	5.25E-03
Eutrophication terrestrial [mol N eq.]	8.65E-02	6.03E-02	5.25E-02
Human toxicity, cancer effect [CTUh]	5.67E-08	5.58E-08	5.55E-08
Human toxicity, non-cancer effects [CTUh]	3.24E-07	3.19E-07	3.18E-07
Ionising radiation [kg U235 eq.]	1.39E+00	1.38E+00	1.38E+00
Ozone depletion [CFC-11]	3.72E-08	3.72E-08	3.72E-08
Particulate matter [kg $PM_{2.5}$ eq.]	1.76E-03	1.43E-03	1.32E-03
Photochemical ozone formation [kg NMVOC]	2.26E-02	1.59E-02	1.38E-02
Resource depletion - mineral fossil and renewable [kg Sb eq.]	2.87E-02	2.67E-02	2.61E-02
Resource deletion – water [m^3 water]	7.81E-05	7.68E-05	7.63E-05

Table S9 - Environmental impacts of 1 kg formate produced via electrochemical reduction for different partition factors (PF) based on the market value of carbon dioxide. The other parameters are: recycling rate at 99.9%, current electricity mix (2020) and a purification thermal energy demand of 35 MJ/kg of formate.

Impact categories	Carbon dioxide flow as a waste to be treated and disposed of			Carbon dioxide flow as a product with a market value		
	PF 80%	***PF 90%***	***PF 95%***	***PF 10%***	***PF 50%***	***PF 90%***
Acidification [mol H^+ eq.]	2.17E-02	2.44E-02	2.58E-02	2.72E-02	2.74E-02	2.76E-02
Climate change [kg CO_2 eq.]	6.57E+00	7.39E+00	7.80E+00	8.22E+00	8.27E+00	8.32E+00
Ecotoxicity freshwater [CTUe]	4.20E+00	4.73E+00	4.99E+00	5.26E+00	5.30E+00	5.35E+00
Eutrophication freshwater [kg P eq.]	1.49E-04	1.68E-04	1.77E-04	1.87E-04	1.89E-04	1.91E-04
Eutrophication marine [kg N eq.]	4.77E-03	5.37E-03	5.67E-03	5.99E-03	6.06E-03	6.13E-03
Eutrophication terrestrial [mol N eq.]	4.83E-02	5.44E-02	5.74E-02	6.06E-02	6.15E-02	6.24E-02
Human toxicity, cancer effect [CTUh]	4.47E-08	5.02E-08	5.30E-08	5.63E-08	5.82E-08	6.02E-08
Human toxicity, non-cancer effects [CTUh]	2.56E-07	2.88E-07	3.04E-07	3.20E-07	3.22E-07	3.24E-07
Ionising radiation [kg U235 eq.]	1.11E+00	1.24E+00	1.31E+00	1.38E+00	1.38E+00	1.39E+00
Ozone depletion [CFC-11]	2.98E-08	3.35E-08	3.54E-08	3.81E-08	4.16E-08	4.51E-08
Particulate matter [kg $PM_{2.5}$ eq.]	1.14E-03	1.28E-03	1.35E-03	1.43E-03	1.44E-03	1.44E-03
Photochemical ozone formation [kg NMVOC]	1.27E-02	1.43E-02	1.51E-02	1.59E-02	1.62E-02	1.65E-02
Resource depletion - mineral fossil and renewable [kg Sb eq.]	2.14E-02	2.40E-02	2.54E-02	2.70E-02	2.80E-02	2.89E-02
Resource deletion – water [m^3 water]	6.14E-05	6.91E-05	7.29E-05	7.68E-05	7.70E-05	7.72E-05

Table S10 – Environmental impacts of 1 kg formate produced via electrochemical reduction for different electricity grid mixes in the UK. The fixed parameters are: thermal energy requirements for the purification step (35MJ/kg of formate), recycling rate at 99.9%, carbon dioxide with a nil market value.

Impact categories	Electricity mix in 2020	Electricity mix in 2030	Electricity mix in 2050
Acidification [mol H^+ eq.]	2.72E-02	1.73E-02	1.51E-02
Climate change [kg CO_2 eq.]	8.19E+00	5.22E+00	5.00E+00
Ecotoxicity freshwater [CTUe]	5.25E+00	5.22E+00	5.20E+00
Eutrophication freshwater [kg P eq.]	1.87E-04	1.89E-04	1.87E-04
Eutrophication marine [kg N eq.]	5.96E-03	3.89E-03	3.38E-03
Eutrophication terrestrial [mol N eq.]	6.03E-02	3.75E-02	3.21E-02
Human toxicity, cancer effect [CTUh]	5.58E-08	5.56E-08	5.44E-08
Human toxicity, non-cancer effects [CTUh]	3.19E-07	3.17E-07	2.32E-07
Ionising radiation [kg U235 eq.]	1.38E+00	1.47E+00	1.56E+00
Ozone depletion [CFC-11]	3.72E-08	3.72E-08	3.72E-08
Particulate matter [kg $PM_{2.5}$ eq.]	1.43E-03	9.97E-04	9.09E-04
Photochemical ozone formation [kg NMVOC]	1.59E-02	1.01E-02	8.65E-03
Resource depletion - mineral fossil and renewable [kg Sb eq.]	2.67E-02	2.41E-02	2.18E-02
Resource deletion – water [m^3 water]	7.68E-05	7.93E-05	8.01E-05

Table S5 –Environmental impacts of 1 kg of formate produced via methyl formate route.

Impact categories	Conventional process
Acidification [mol H^+ eq.]	1.53E-02
Climate change [kg CO_2 eq.]	2.94E+00
Ecotoxicity freshwater [CTUe]	9.23E+00
Eutrophication freshwater [kg P eq.]	5.98E-04
Eutrophication marine [kg N eq.]	1.95E-03
Eutrophication terrestrial [mol N eq.]	2.12E-02
Human toxicity, cancer effect [CTUh]	9.06E-08
Human toxicity, non-cancer effects [CTUh]	4.58E-07
Ionising radiation [kg U235 eq.]	2.17E-01
Ozone depletion [CFC-11]	4.60E-07
Particulate matter [kg $PM_{2.5}$ eq.]	1.09E-03
Photochemical ozone formation [kg NMVOC]	6.83E-03
Resource depletion - mineral fossil and renewable [kg Sb eq.]	8.42E-02
Resource deletion – water [m^3 water]	3.85E-05

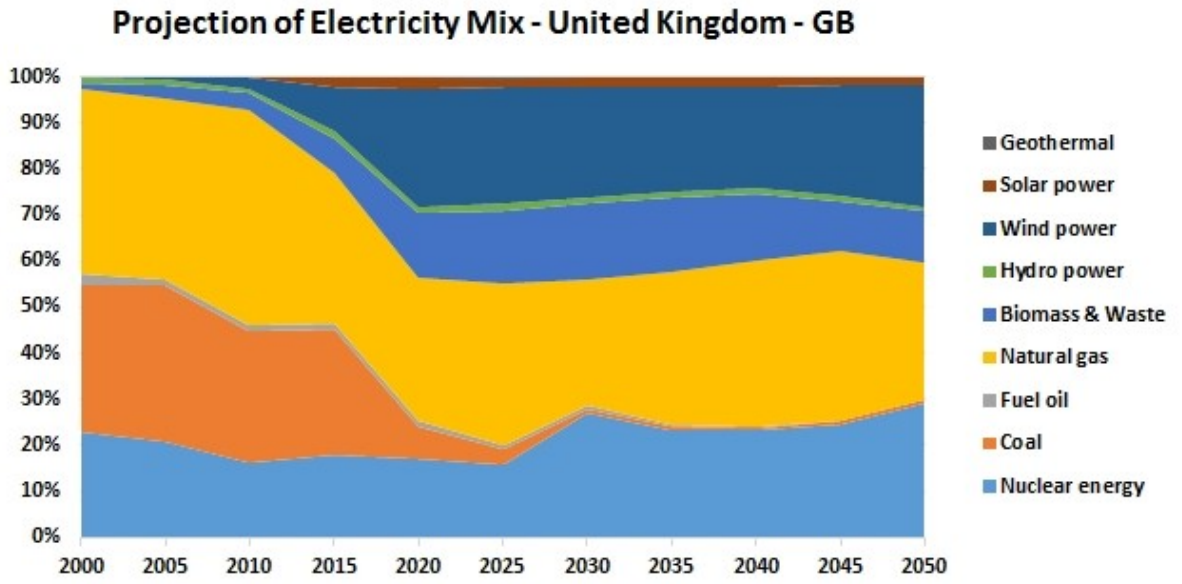

Figure S1 – Chart from GaBi documentation* reporting the various source contribution to the electricity mixes in the United Kingdom from 2000 to 2050. Percentages were estimated from the "EU Reference Scenario 2016. Energy, transport and GHG emissions. Trends to 2050" (European Commission, 2016).

*http://gabi-documentation-2021.gabi-software.com/xml-data/sources/a1487940-b6ea-4f7b-97b6-6f1f72fed90f.xml

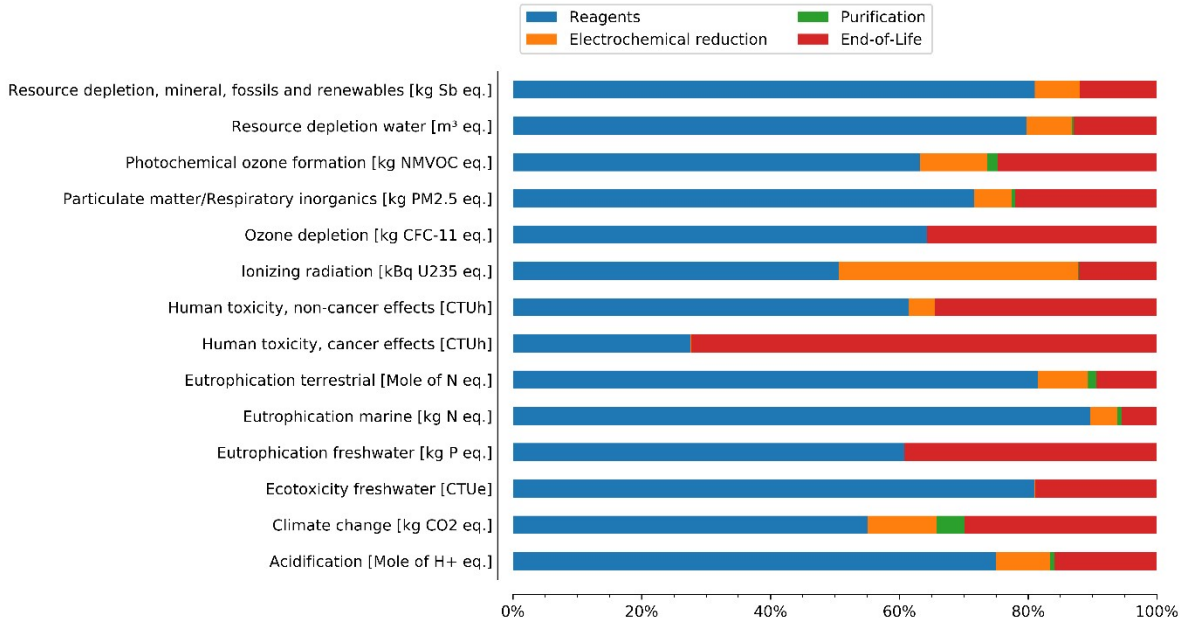

Figure S2 - Hot-spot analysis for the baseline scenario and recycling rate of 95%.

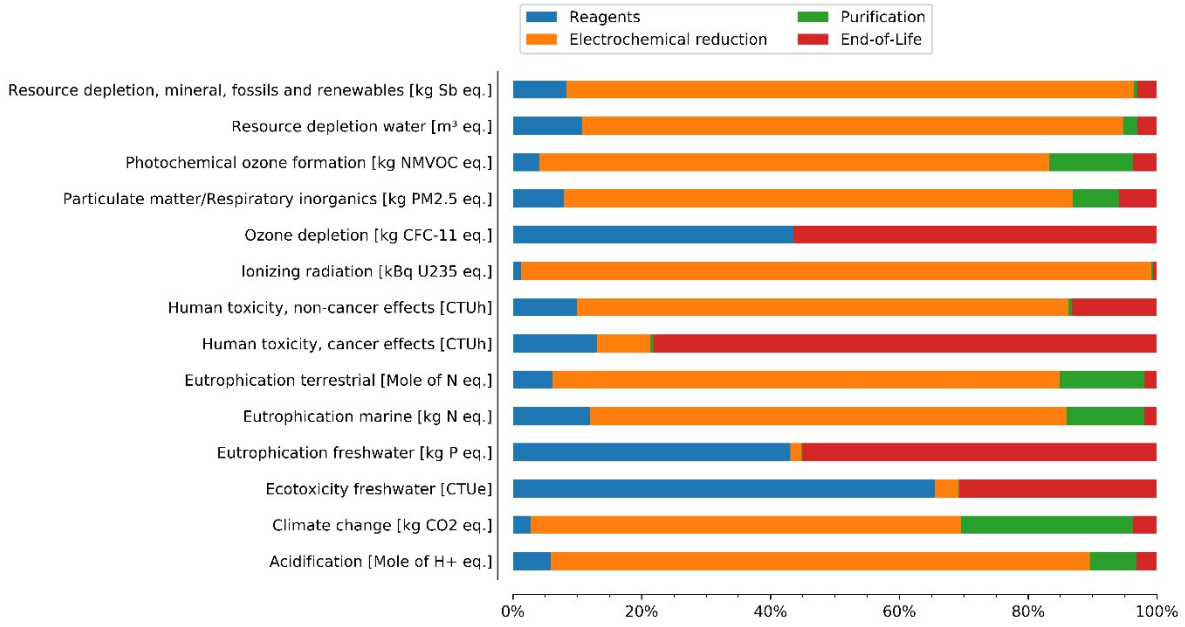

Figure S3 - Hot-spot analysis for the baseline scenario and recycling rate of 99.9%.

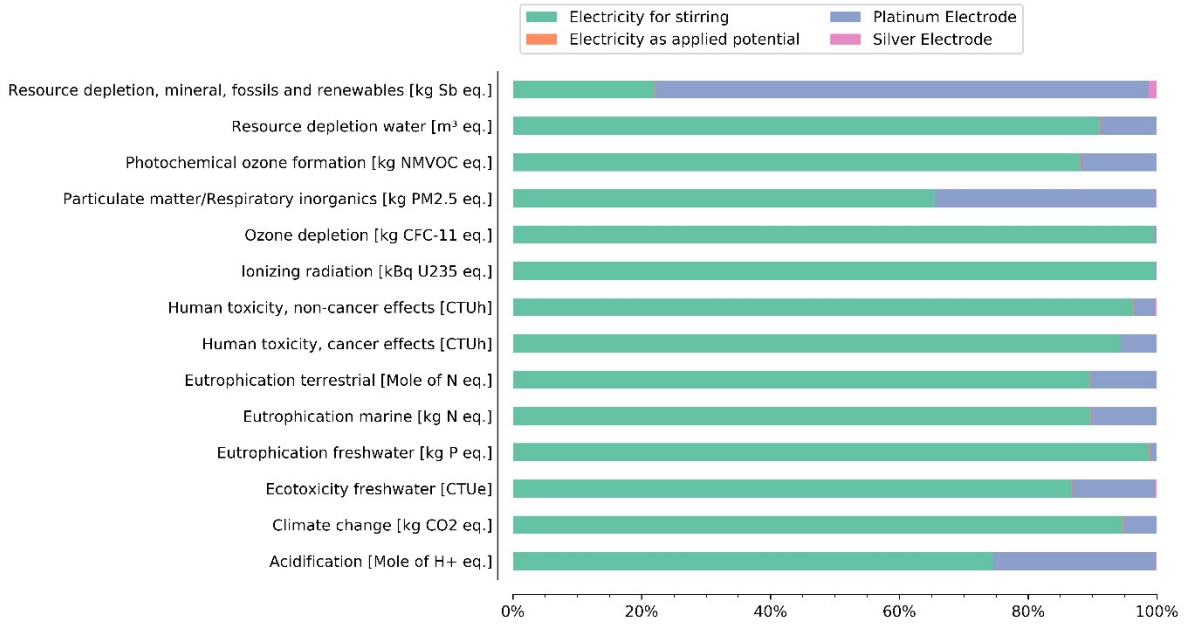

Figure S4 - Detailed hot-spot analysis for electrochemical reduction

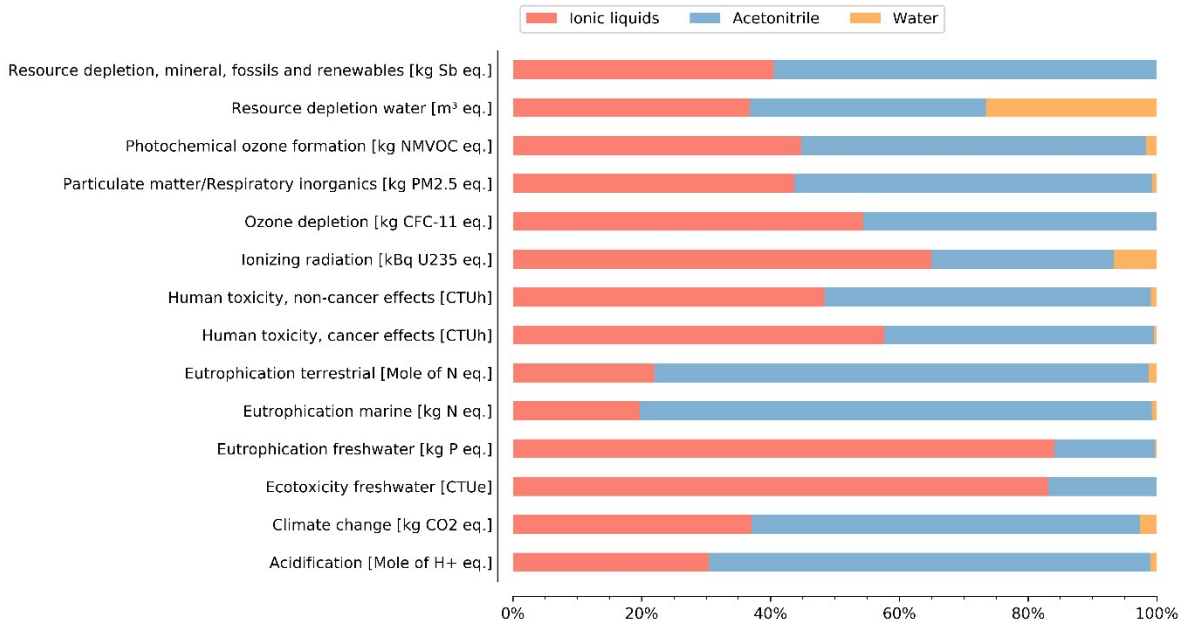

Figure S5 - Detailed hot-spot analysis for reagents