Comparative gate-to-gate life cycle assessment for the alkali and acid pre-treatment step in the chemical recycling of waste cotton – Electronic supplementary material

Lucas Rosson[1,*] & Nolene Byrne[1]

Institute for Frontier Materials, Deakin University, 75 Pigdons Road, Waurn Ponds VIC 3216, Australia.[1]

*Corresponding author, email: lrosson@deakin.edu.au

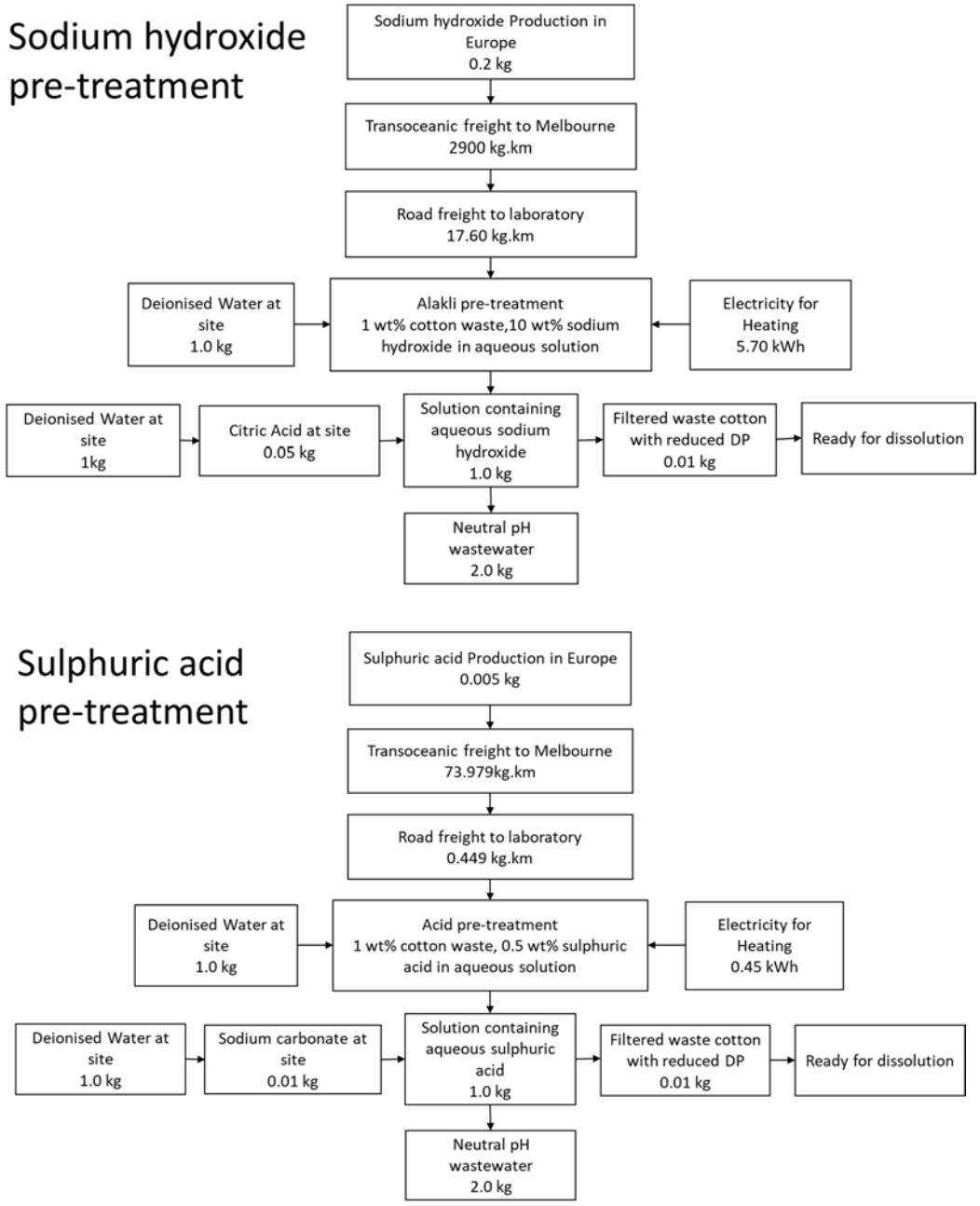

Figure S1. Diagram of flows for each pre-treatment process.

Deionised water
The cotton waste is required to be pre-treated at 1 wt% consistency in solution, therefore the amount of deionised water required for the pre-treatment solution for both process 1 and process 2 was 1 kg. The amount required for washing in both processes was also 1 kg, therefore a total of 2 kg of deionised water was used for each process. This data was obtained from the AusLCI database in SimaPro. The deionised water was assumed to be produced onsite and therefore no transportation was allocated.

Sodium hydroxide for process 1
To form an aqueous solution of 10 wt% sodium hydroxide, 0.1 kg of sodium hydroxide is required per functional unit. The sodium hydroxide was assumed to be produced in Europe, approximately 14,500 km from Melbourne. From here it was transported via transoceanic freight to Melbourne, after which it was transported by a 5 tonne truck to our laboratory, which is approximately 90km from Melbourne. Due to this chemical being produced as 50% sodium hydroxide in aqueous solution, the amount required to be transported was 0.2 kg per functional unit. Inventory for both production and transport of sodium hydroxide was found in the AusLCI database. The input value for the sodium hydroxide production was 0.2 kg. The input values for sodium hydroxide transoceanic freight and transport by truck were found by multiplying the amount required in kilograms by the distance travelled, yielding 2900 kg.km and 17.60 kg.km, respectively.

Sulphuric acid for process 2
To form an aqueous solution of 0.5 wt% sulphuric acid, approximately 0.005 kg per functional unit is required. The sulphuric acid was assumed to be produced at the same location as the sodium hydroxide and thus was subject to an identical transportation route. Again, the data for sulphuric acid production and transport was obtained from the AusLCI database. The input value for the sulphuric acid production was 0.005 kg. The input values for sulphuric acid transoceanic freight and transport by truck were found by multiplying the amount required in kilograms by the distance travelled, yielding 72.5 kg.km and 0.45 kg.km, respectively.

Electricity use
For process 1, the amount of electricity required was calculated to be approximately 5.70 kWh. For process 2, the amount of electricity required was 0.45 kWh. It was observed that the heat-up time was approximately 12 minutes for both processes and assumed that the heating system ran at an average of half of the devices' rated power for the duration of the heating. The equation used for heating energy can be found below:

$$E_{elec} = (0.2 + t_{process})P_{avg}$$

Where E_{elec} is the energy for heating in kilo-watt hours; $t_{process}$ is the processing time at final temperature; and P_{avg} is the average power of the heating device (375 W, assumed from rated power). The time at final temperature was 15 hours for process 1, and 1 hour for process 2. The electricity was sourced from the Victorian/Australian grid mix, for which data was available in the AusLCI database.

Citric acid for process 1 neutralisation
For neutralisation of the alkali pre-treatment solution, it was observed through experimentation that approximately 0.05 kg of citric acid was required. The citric acid was assumed to be produced onsite and thus had no transportation allocated. The data for production of citric acid was obtained from the AusLCI database.

Sodium carbonate for process 2 neutralisation
For neutralisation of the acid pre-treatment solution, approximately 0.01 kg was required. The sodium carbonate was assumed to be produced onsite and thus had no transportation allocated. The data for production of sodium carbonate was obtained from the AusLCI database.

Flow	Input	Function	Value	Units
P1.1	Sodium hydroxide, 50% in H2O, production mix, at plant/kg/RER	Manufacture of sodium hydroxide in Europe	200	g
P1.2	Transport, transoceanic freight ship	Transport of chemical from Europe to Melbourne	2900	kgkm
P1.3	Transport, truck, 5-16t, fleet average	Transport of chemical from Melbourne to Laboratory	17.6	kgkm
P1.4	Electricity mix, Victoria	Electricity used in treatment process	5.70	kWh
P1.5	Citric acid [GLO] | market for | APOS, U	Neutralisation of sodium hydroxide solution	0.05	kg
P1.6	Water, deionised, at plant	Treatment water and washing water	2	kg

Flow	Input	Function	Value	Units
P2.1	Sulfuric acid, liquid, at plant/RER U/AusSD U	Manufacture of sulfuric acid in Europe	5.0	g
P2.2	Transport, transoceanic freight ship	Transport of chemical from Europe to Melbourne	73.979	kgkm
P2.3	Transport, truck, 5-16t, fleet average	Transport of chemical from Melbourne to Laboratory	0.449	Kgkm
P2.4	Electricity mix, Victoria	Electricity used in treatment process	0.45	kWh
P2.5	Sodium carbonate from ammonium chloride production, at plant/GLO U/ AusSD U	Neutralisation of sulfuric acid solution	0.01	kg
P2.6	Water, deionised, at plant	Treatment water and washing water	2	kg

Table S1. Description of flows for each process and accompanying tables.

Flow	Type	Specification	Units	Total	Sodium hydroxide production	Citric acid production	Water, deionised	Electricity consumption	transport via truck	Transport via transoceanic freight ship
Input	Raw	Carbon dioxide, in air	g	1.90E+02	4.39E+00	1.47E+02	1.17E-01	3.87E+01	3.00E-02	8.94E-02
		Cadmium	g	5.13E-03	6.79E-05	4.59E-03	7.27E-07	4.56E-04	2.00E-05	1.62E-06
		Clay, unspecified	g	9.53E+00	4.49E+00	4.61E+00	2.93E-02	3.77E-01	1.54E-02	8.72E-03
		Coal, 18.0 MJ per kg, in ground	g	7.32E+01	6.52E+01	0.00E+00	6.45E-01	5.22E+00	4.40E-01	1.75E+00
		Coal, 26.4 MJ per kg	g	4.71E+01	4.21E+01	0.00E+00	4.06E-01	3.13E+00	2.86E-01	1.14E+00
		Coal, brown	g	1.13E+01	1.06E-02	1.12E+01	1.22E-04	4.22E-03	4.88E-04	8.96E-04
		Coal, brown, 10.0 MJ per kg, in ground	g	6.49E+03	1.12E+02	0.00E+00	1.07E+00	6.37E+03	6.00E-01	2.86E+00
		Coal, hard	g	8.05E+01	4.08E-02	8.03E+01	1.64E-03	1.33E-01	1.09E-03	1.29E-03
		Energy, geothermal, converted	MJ	2.38E-03	0.00E+00	2.38E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00
		Energy, gross calorific value, in biomass	MJ	1.65E+00	2.57E-02	1.60E+00	9.39E-04	1.91E-02	2.09E-04	3.53E-04
		Energy, gross calorific value, in biomass, primary forest	MJ	2.23E-03	1.34E-06	2.23E-03	1.47E-08	2.11E-06	4.27E-07	5.27E-07
		Energy, kinetic (in wind), converted	MJ	1.55E+00	9.03E-02	1.94E-02	1.39E-03	1.43E+00	4.73E-04	2.32E-03
		Energy, potential (in hydropower reservoir), converted	MJ	1.65E+00	1.19E-01	1.04E-01	1.13E-03	1.43E+00	6.60E-04	2.95E-03
		Energy, solar, converted	MJ	6.36E-01	6.47E-02	4.13E-04	6.20E-04	5.68E-01	3.40E-04	1.66E-03
		Gas, mine, off-gas, process, coal mining/m3	m3	7.34E-04	1.11E-07	7.34E-04	5.94E-09	1.51E-07	6.68E-09	5.64E-09
		Gas, natural, 36.6 MJ per m3	m3	3.31E-02	1.32E-02	0.00E+00	1.42E-04	1.93E-02	1.85E-04	3.55E-04
		Gas, natural/m3	m3	2.52E-02	1.39E-03	2.29E-02	2.29E-05	4.85E-04	8.69E-05	3.71E-04
		Gravel	g	1.38E+02	2.39E+01	4.13E+01	1.13E+00	6.41E+01	6.48E+00	5.84E-01
		Iron	g	8.37E+00	1.63E+00	2.92E+00	4.12E-02	3.15E+00	2.75E-01	3.46E-01
		Land occupation	m2a	1.37E-01	3.44E-02	8.51E-02	7.46E-04	1.54E-02	3.74E-04	9.23E-04

		Lead	g	9.53E-02	8.03E-03	7.64E-02	7.88E-05	7.94E-03	2.60E-03	2.15E-04
		Oil, crude	g	3.27E+01	4.05E+00	1.62E+01	9.11E-02	2.79E+00	1.58E+00	7.92E+00
		Oxygen	g	4.54E+03	2.38E+02	1.88E+00	2.29E+00	4.29E+03	1.28E+00	6.09E+00
		Potassium chloride	g	1.22E+00	3.28E-03	1.21E+00	2.89E-05	4.21E-03	4.04E-05	7.23E-05
		Shale	g	1.45E+01	1.73E-06	1.45E+01	2.54E-07	3.24E-06	6.95E-08	5.98E-08
		Sodium chloride	g	1.95E+02	1.69E+02	2.53E+01	6.50E-01	2.94E-01	6.26E-02	9.05E-03
		Tellurium	g	1.42E-02	2.65E-03	4.08E-07	1.90E-05	1.15E-02	3.10E-05	3.40E-05
		Land transformation	m2	1.99E-01	9.61E-04	1.97E-01	1.64E-05	5.82E-04	1.74E-05	5.14E-05
		Volume occupied, final repository for low-active radioactive waste	m3	2.90E-09	1.20E-11	2.87E-09	1.23E-13	1.23E-11	1.54E-13	2.42E-13
		Volume occupied, final repository for radioactive waste	m3	1.55E-10	3.01E-12	1.49E-10	2.98E-14	3.02E-12	3.78E-14	6.06E-14
		Volume occupied, reservoir	m3day	2.25E+01	1.61E+00	3.93E-01	1.54E-02	2.04E+01	8.73E-03	4.11E-02
		Volume occupied, underground deposit	m3	2.06E-08	1.23E-08	2.77E-09	4.02E-11	5.29E-09	8.57E-11	1.19E-10
		Water, cooling	m3	2.70E-02	1.42E-02	1.20E-11	4.11E-14	6.55E-13	1.38E-14	3.75E-14
		Water, lake	m3	3.53E-04	1.94E-07	3.53E-04	2.03E-09	1.94E-07	2.65E-08	2.89E-09
		Water, river	m3	1.29E-02	6.28E-05	1.28E-02	6.53E-07	4.98E-05	1.65E-06	6.90E-06
		Water, salt	m3	8.11E-05	8.04E-06	5.68E-05	1.33E-07	5.70E-06	1.63E-06	8.78E-06
		Water, turbine use	m3	1.71E+00	3.23E-01	9.18E-01	3.01E-03	4.57E-01	1.91E-03	7.32E-03
		Water, unspecified natural origin	m3	1.49E-02	1.80E-03	3.33E-04	2.23E-03	1.04E-02	2.05E-05	4.10E-05
		Water, well	m3	1.26E-02	8.82E-06	1.26E-02	7.90E-08	2.42E-06	2.56E-06	6.69E-07
		Wood	m3	1.66E-05	2.26E-06	1.30E-05	7.38E-08	1.31E-06	1.71E-08	2.28E-08
Output	Air	Ammonia	g	1.82E-01	8.62E-03	1.48E-01	5.47E-05	2.23E-02	7.75E-05	3.01E-03
		Nitrogen oxides	g	1.18E+01	1.02E+00	7.54E-01	1.16E-02	9.52E+00	3.70E-02	4.31E-01
		Sulfur dioxide	g	1.72E+00	9.33E-02	1.18E+00	1.35E-03	6.31E-02	6.75E-03	3.77E-01
		Carbon dioxide, fossil	g	6.59E+03	3.54E+02	2.66E+02	3.66E+00	5.93E+03	6.54E+00	3.40E+01
		Dinitrogen monoxide	g	1.45E-01	6.23E-03	5.13E-02	7.21E-05	8.63E-02	1.34E-04	7.75E-04
		Methane, fossil	g	1.18E+00	6.98E-02	8.04E-01	9.42E-04	2.90E-01	3.64E-03	1.41E-02
		Chromium VI	g	6.37E-05	1.08E-05	1.18E-05	1.01E-07	4.09E-05	4.39E-08	7.57E-08

		Methane, bromochlorodifluoro-, Halon 1211	g	9.09E-07	9.60E-10	9.06E-07	1.64E-11	4.84E-10	2.76E-10	1.38E-09
		Methane, bromotrifluoro-, Halon 1301	g	1.45E-06	1.48E-07	8.68E-07	2.99E-09	1.03E-07	5.92E-08	2.72E-07
		Methane, tetrachloro-, CFC-10	g	2.57E-05	2.69E-06	2.15E-05	9.26E-07	5.09E-07	5.27E-09	6.00E-09
		Carbon monoxide	g	1.77E+00	1.54E-01	0.00E+00	3.30E-03	1.58E+00	3.28E-02	3.77E-03
		Carbon monoxide, fossil	g	6.95E-01	9.25E-02	4.12E-01	1.80E-03	1.16E-01	9.21E-03	6.44E-02
		Mercury	g	2.87E-04	1.24E-04	9.15E-06	4.00E-07	1.53E-04	3.48E-07	8.02E-07
	Water	Nitrate	g	1.78E+00	7.15E-02	1.36E+00	4.06E-04	3.52E-01	2.63E-04	6.52E-04
		Phosphate	g	4.64E-01	8.45E-02	3.26E-01	6.28E-04	5.05E-02	8.63E-04	1.32E-03
		Beryllium	g	3.40E-03	4.39E-04	2.47E-04	4.04E-06	2.69E-03	2.63E-06	1.03E-05
		Nickel	g	4.32E-02	5.67E-03	9.07E-03	5.92E-05	2.82E-02	5.27E-05	1.46E-04
		Vanadium	g	2.00E-02	2.48E-03	1.62E-03	2.75E-05	1.58E-02	2.59E-05	7.11E-05
		Thallium	g	1.59E-03	2.11E-04	7.05E-05	2.00E-06	1.30E-03	1.25E-06	4.97E-06
		Barium	g	3.14E-01	3.70E-02	1.01E-02	3.54E-04	2.65E-01	2.78E-04	1.37E-03
	Soil	Chromium VI	g	5.15E-04	4.53E-04	1.75E-05	4.33E-06	2.62E-05	2.35E-06	1.18E-05
		Cypermethrin	g	4.02E-06	2.16E-09	4.01E-06	2.36E-11	3.40E-09	6.87E-10	8.50E-10

Table S2. Life cycle inventory for sodium hydroxide pre-treatment process.

Flow	Type	Specification	Units	Total	Sulfuric acid production	Sodium carbonate production	Water, deionised	Electricity consumption	Transport via truck	Transport via transoceanic freight ship
Input	Raw	Calcite	g	1.24E+00	3.19E-02	3.80E-01	2.19E-01	5.98E-01	5.66E-03	4.48E-03
		Carbon dioxide, in air	g	3.33E+00	1.53E-02	1.35E-01	1.17E-01	3.06E+00	7.65E-04	2.28E-03
		Clay, unspecified	g	4.41E-01	5.35E-02	3.27E-01	2.93E-02	2.98E-02	3.93E-04	2.22E-04
		Coal, 18.0 MJ per kg, in ground	g	2.34E+00	6.21E-02	1.17E+00	6.45E-01	4.12E-01	1.12E-02	4.47E-02
		Coal, 26.4 MJ per kg	g	1.49E+00	4.02E-02	7.58E-01	4.06E-01	2.47E-01	7.31E-03	2.91E-02

Coal, brown, 10.0 MJ per kg, in ground	g	5.06E+02	9.60E-02	1.95E+00	1.07E+00	5.03E+02	1.53E-02	7.29E-02
Gravel	g	8.24E+00	2.41E-01	1.63E+00	1.13E+00	5.06E+00	1.65E-01	1.49E-02
Oil, crude	g	1.48E+00	1.27E-01	8.02E-01	9.11E-02	2.20E-01	4.03E-02	2.02E-01
Oxygen	g	3.46E+02	2.01E-01	4.14E+00	2.29E+00	3.39E+02	3.25E-02	1.55E-01
Sodium chloride	g	6.48E+00	1.62E-03	5.81E+00	6.50E-01	2.32E-02	1.60E-03	2.31E-04
Energy, gross calorific value, in biomass	MJ	3.86E-03	1.75E-04	1.22E-03	9.39E-04	1.51E-03	5.33E-06	8.99E-06
Energy, gross calorific value, in biomass, primary forest	MJ	3.45E-07	2.81E-08	1.11E-07	1.47E-08	1.67E-07	1.09E-08	1.35E-08
Energy, kinetic (in wind), converted	MJ	1.16E-01	7.41E-05	1.56E-03	1.39E-03	1.13E-01	1.21E-05	5.91E-05
Energy, potential (in hydropower reservoir), converted	MJ	1.16E-01	1.56E-04	2.38E-03	1.13E-03	1.13E-01	1.68E-05	7.54E-05
Energy, solar, converted	MJ	4.67E-02	5.33E-05	1.12E-03	6.20E-04	4.48E-02	8.69E-06	4.23E-05
Gas, mine, off-gas, process, coal mining/m3	m3	2.45E-08	8.26E-10	5.51E-09	5.94E-09	1.19E-08	1.70E-10	1.44E-10
Gas, natural, 36.6 MJ per m3	m3	3.65E-03	1.80E-05	1.95E-03	1.42E-04	1.52E-03	4.73E-06	9.05E-06
Gas, natural/m3	m3	1.38E-04	6.99E-06	5.78E-05	2.29E-05	3.83E-05	2.22E-06	9.46E-06
land occupation	m2a	3.34E-03	1.46E-04	1.19E-03	7.46E-04	1.22E-03	9.55E-06	2.35E-05
land transformation	m2	1.22E-04	7.47E-06	5.05E-05	1.64E-05	4.60E-05	4.45E-07	1.31E-06
Volume occupied, final repository for low-active radioactive waste	m3	2.01E-12	1.18E-13	7.83E-13	1.23E-13	9.73E-13	3.92E-15	6.17E-15
Volume occupied, final repository for radioactive waste	m3	4.98E-13	2.98E-14	1.97E-13	2.98E-14	2.38E-13	9.64E-16	1.55E-15
Volume occupied, reservoir	m3day	1.66E+00	1.42E-03	2.83E-02	1.54E-02	1.61E+00	2.23E-04	1.05E-03
Volume occupied, underground deposit	m3	5.63E-10	1.27E-11	8.74E-11	4.02E-11	4.17E-10	2.19E-12	3.04E-12
Water, cooling, unspecified natural origin/m3	m3	4.17E-04	5.30E-06	3.18E-04	4.11E-05	5.17E-05	3.51E-07	9.57E-07
Water, lake	m3	2.88E-08	1.34E-09	9.35E-09	2.03E-09	1.53E-08	6.77E-10	7.38E-11

		Water, river	m3	8.39E-06	1.04E-06	2.54E-06	6.53E-07	3.93E-06	4.21E-08	1.76E-07
		Water, unspecified natural origin	m3	3.37E-03	2.46E-04	6.26E-05	2.23E-03	8.24E-04	5.24E-07	1.05E-06
		Water, well	m3	9.89E-07	7.28E-08	5.63E-07	7.90E-08	1.91E-07	6.53E-08	1.71E-08
		Wood, various	m3	3.18E-07	1.83E-08	1.22E-07	7.38E-08	1.03E-07	4.35E-10	5.81E-10
		Copper, 1.18% in sulfide, Cu 0.39% and Mo 8.2E-3% in crude ore	g	8.83E-03	6.42E-04	4.60E-03	8.17E-04	2.71E-03	2.03E-05	4.06E-05
		Copper, 2.19% in sulfide, Cu 1.83% and Mo 8.2E-3% in crude ore	g	1.18E-02	8.54E-04	6.11E-03	1.08E-03	3.68E-03	2.70E-05	5.35E-05
		Tellurium	g	1.07E-06	1.74E-08	1.22E-07	1.90E-08	9.07E-07	7.91E-10	8.67E-10
Output	Air	Ammonia	g	5.59E-03	2.70E-05	3.68E-03	5.47E-05	1.76E-03	1.98E-06	7.68E-05
		Nitrogen oxides	g	8.05E-01	4.58E-03	2.57E-02	1.16E-02	7.51E-01	9.45E-04	1.10E-02
		Sulfur dioxide	g	9.06E-02	6.40E-02	1.05E-02	1.35E-03	4.98E-03	1.72E-04	9.61E-03
		Carbon dioxide, fossil	g	4.85E+02	7.21E-01	1.18E+01	3.66E+00	4.68E+02	1.67E-01	8.67E-01
		Dinitrogen monoxide	g	7.10E-03	1.14E-05	1.78E-04	7.21E-05	6.81E-03	3.42E-06	1.98E-05
		Methane, fossil	g	4.96E-02	2.99E-04	2.50E-02	9.42E-04	2.29E-02	9.29E-05	3.59E-04
		Chromium VI	g	4.11E-06	1.06E-07	6.78E-07	1.01E-07	3.23E-06	1.12E-09	1.93E-09
		Methane, bromotrifluoro-, Halon 1301	g	5.20E-08	4.42E-09	2.80E-08	2.99E-09	8.13E-09	1.51E-09	6.94E-09
		Methane, chlorodifluoro-, HCFC-22	g	7.23E-07	4.00E-09	3.61E-08	1.47E-08	6.67E-07	2.65E-10	7.07E-10
		Methane, tetrachloro-, CFC-10	g	9.74E-07	9.21E-10	6.14E-09	9.26E-07	4.02E-08	1.35E-10	1.53E-10
		Carbon monoxide	g	1.33E-01	3.67E-04	3.98E-03	3.30E-03	1.25E-01	8.37E-04	9.62E-05
		Carbon monoxide, fossil	g	1.96E-02	8.56E-04	5.87E-03	1.80E-03	9.15E-03	2.35E-04	1.64E-03
		Mercury	g	1.28E-05	3.51E-08	2.70E-07	4.00E-07	1.21E-05	8.87E-09	2.05E-08
	Water	Ammonium, ion	g	4.72E-02	1.36E-05	4.09E-02	6.70E-05	6.23E-03	1.02E-06	3.13E-06
		Phosphate	g	9.31E+00	5.48E-01	4.09E+00	6.28E-01	3.99E+00	2.20E-02	3.36E-02
		Beryllium	g	2.28E-04	8.16E-07	9.92E-06	4.04E-06	2.13E-04	6.70E-08	2.63E-07
		Nickel	g	2.51E-03	2.35E-05	1.95E-04	5.92E-05	2.23E-03	1.34E-06	3.72E-06
		Vanadium	g	1.34E-03	4.60E-06	5.55E-05	2.75E-05	1.25E-03	6.60E-07	1.81E-06

	Thallium	g	1.10E-04	3.82E-07	4.71E-06	2.00E-06	1.03E-04	3.20E-08	1.27E-07
	Barium	g	2.20E-02	3.94E-05	6.82E-04	3.54E-04	2.09E-02	7.09E-06	3.50E-05
Soil	Chromium VI	g	1.48E-05	3.47E-07	7.73E-06	4.33E-06	2.07E-06	6.00E-08	3.00E-07

Table S3. Life cycle inventory for sulphuric acid pre-treatment process.

Impact category	Unit	Total	Sodium hydroxide production	Citric acid production	Water, deionised	Electricity consumption	transport via truck	Transport via transoceanic freight ship
Abiotic depletion	kg Sb eq	4.75E-06	1.35E-06	2.18E-06	9.10E-09	1.17E-06	3.60E-08	1.20E-08
Abiotic depletion (fossil fuels)	MJ	6.32E+00	1.82E+00	3.07E+00	2.07E-02	9.27E-01	8.57E-02	3.98E-01
Global warming (GWP100a)	kg CO2 eq	6.70E+00	3.68E-01	3.07E-01	3.83E-03	5.98E+00	6.82E-03	3.49E-02
Ozone layer depletion (ODP)	kg CFC-11 eq	4.67E-08	3.90E-09	3.57E-08	7.14E-10	2.45E-09	7.17E-10	3.28E-09
Human toxicity	kg 1,4-DB eq	1.11E+00	1.64E-01	1.53E-01	1.53E-03	7.81E-01	1.30E-03	1.08E-02
Fresh water aquatic ecotox.	kg 1,4-DB eq	8.33E-01	1.11E-01	1.06E-01	1.08E-03	6.12E-01	8.75E-04	2.87E-03
Marine aquatic ecotoxicity	kg 1,4-DB eq	2.69E+03	3.37E+02	3.62E+02	3.16E+00	1.97E+03	2.50E+00	1.09E+01
Terrestrial ecotoxicity	kg 1,4-DB eq	1.24E-02	6.47E-03	9.55E-04	3.96E-05	4.79E-03	2.61E-05	1.19E-04
Photochemical oxidation	kg C2H4 eq	1.83E-04	1.68E-05	8.48E-05	3.93E-07	5.86E-05	1.70E-06	2.10E-05
Acidification	kg SO2 eq	8.26E-03	6.42E-04	2.03E-03	7.59E-06	4.88E-03	2.68E-05	6.73E-04
Eutrophication	kg PO4--- eq	2.48E-03	2.48E-04	6.85E-04	2.40E-06	1.47E-03	6.32E-06	6.16E-05

Table S4. Impact category characterisation values for sodium hydroxide process with the main contributing process component highlighted.

Impact category	Unit	Total	Sulfuric acid production	Sodium carbonate production	Water, deionised	Electricity consumption	transport via truck	Transpor via transoceanic freight ship
Abiotic depletion	kg Sb eq	1.91E-07	1.18E-08	7.69E-08	9.10E-09	9.24E-08	9.20E-10	3.07E-10
Abiotic depletion (fossil fuels)	MJ	2.42E-01	7.47E-03	1.28E-01	2.07E-02	7.32E-02	2.19E-03	1.01E-02
Global warming (GWP100a)	kg CO2 eq	4.91E-01	7.51E-04	1.29E-02	3.83E-03	4.72E-01	1.74E-04	8.90E-04
Ozone layer depletion (ODP)	kg CFC-11 eq	1.41E-09	5.44E-11	3.47E-10	7.14E-10	1.93E-10	1.83E-11	8.37E-11
Human toxicity	kg 1,4-DB eq	7.20E-02	7.76E-04	7.74E-03	1.53E-03	6.17E-02	3.32E-05	2.75E-04
Fresh water aquatic ecotox.	kg 1,4-DB eq	5.28E-02	3.06E-04	2.98E-03	1.08E-03	4.83E-02	2.23E-05	7.33E-05
Marine aquatic ecotoxicity	kg 1,4-DB eq	1.69E+02	7.82E-01	8.53E+00	3.16E+00	1.56E+02	6.38E-02	2.78E-01
Terrestrial ecotoxicity	kg 1,4-DB eq	4.88E-04	3.86E-06	6.29E-05	3.96E-05	3.78E-04	6.65E-07	3.04E-06
Photochemical oxidation	kg C2H4 eq	9.97E-06	3.13E-06	1.24E-06	3.93E-07	4.63E-06	4.33E-08	5.37E-07
Acidification	kg SO2 eq	5.21E-04	7.91E-05	3.14E-05	7.59E-06	3.85E-04	6.83E-07	1.72E-05
Eutrophication	kg PO4--- eq	1.45E-04	1.24E-06	2.32E-05	2.40E-06	1.16E-04	1.61E-07	1.57E-06

Table S5. Impact category characterization values for sulfuric acid process with the main contributing process component highlighted.

Impact category	Unit	Total	Sodium hydroxide production	Citric acid production	Water, deionised	Transport via truck	Transport via transoceanic freight ship
Abiotic depletion	kg Sb eq	3.58E-06	1.35E-06	2.18E-06	9.10E-09	3.60E-08	1.20E-08
Abiotic depletion (fossil fuels)	MJ	5.40E+00	1.82E+00	3.07E+00	2.07E-02	8.57E-02	3.98E-01
Global warming (GWP100a)	kg CO2 eq	7.21E-01	3.68E-01	3.07E-01	3.83E-03	6.82E-03	3.49E-02
Ozone layer depletion (ODP)	kg CFC-11 eq	4.43E-08	3.90E-09	3.57E-08	7.14E-10	7.17E-10	3.28E-09
Human toxicity	kg 1,4-DB eq	3.30E-01	1.64E-01	1.53E-01	1.53E-03	1.30E-03	1.08E-02
Fresh water aquatic ecotox.	kg 1,4-DB eq	2.21E-01	1.11E-01	1.06E-01	1.08E-03	8.75E-04	2.87E-03
Marine aquatic ecotoxicity	kg 1,4-DB eq	7.16E+02	3.37E+02	3.62E+02	3.16E+00	2.50E+00	1.09E+01
Terrestrial ecotoxicity	kg 1,4-DB eq	7.61E-03	6.47E-03	9.55E-04	3.96E-05	2.61E-05	1.19E-04
Photochemical oxidation	kg C2H4 eq	1.25E-04	1.68E-05	8.48E-05	3.93E-07	1.70E-06	2.10E-05
Acidification	kg SO2 eq	3.38E-03	6.42E-04	2.03E-03	7.59E-06	2.68E-05	6.73E-04
Eutrophication	kg PO4--- eq	1.00E-03	2.48E-04	6.85E-04	2.40E-06	6.32E-06	6.16E-05

Table S6. Impact category characterization values for sodium hydroxide process excluding electricity for heating with the main contributing process component highlighted.

Impact category	Unit	Total	Sulphuric acid production	Sodium carbonate production	Water, deionised	Transport via truck	Transport via transoceanic freight ship
Abiotic depletion	kg Sb eq	9.91E-08	1.18E-08	7.69E-08	9.10E-09	9.20E-10	3.07E-10
Abiotic depletion (fossil fuels)	MJ	1.69E-01	7.47E-03	1.28E-01	2.07E-02	2.19E-03	1.01E-02
Global warming (GWP100a)	kg CO2 eq	1.85E-02	7.51E-04	1.29E-02	3.83E-03	1.74E-04	8.90E-04
Ozone layer depletion (ODP)	kg CFC-11 eq	1.22E-09	5.44E-11	3.47E-10	7.14E-10	1.83E-11	8.37E-11
Human toxicity	kg 1,4-DB eq	1.04E-02	7.76E-04	7.74E-03	1.53E-03	3.32E-05	2.75E-04
Fresh water aquatic ecotox.	kg 1,4-DB eq	4.47E-03	3.06E-04	2.98E-03	1.08E-03	2.23E-05	7.33E-05
Marine aquatic ecotoxicity	kg 1,4-DB eq	1.28E+01	7.82E-01	8.53E+00	3.16E+00	6.38E-02	2.78E-01
Terrestrial ecotoxicity	kg 1,4-DB eq	1.10E-04	3.86E-06	6.29E-05	3.96E-05	6.65E-07	3.04E-06
Photochemical oxidation	kg C2H4 eq	5.34E-06	3.13E-06	1.24E-06	3.93E-07	4.33E-08	5.37E-07
Acidification	kg SO2 eq	1.36E-04	7.91E-05	3.14E-05	7.59E-06	6.83E-07	1.72E-05
Eutrophication	kg PO4--- eq	2.85E-05	1.24E-06	2.32E-05	2.40E-06	1.61E-07	1.57E-06

Table S7. Impact category characterization values for sulphuric acid process excluding electricity for heating with the main contributing process component highlighted.