Supplementary Information (SI) for Green Chemistry.

Supplementary Information

Assessments of life cycle and biodegradation properties uncovered distinct profiles of pharmaceutical excipients guiding selection for drug formulations

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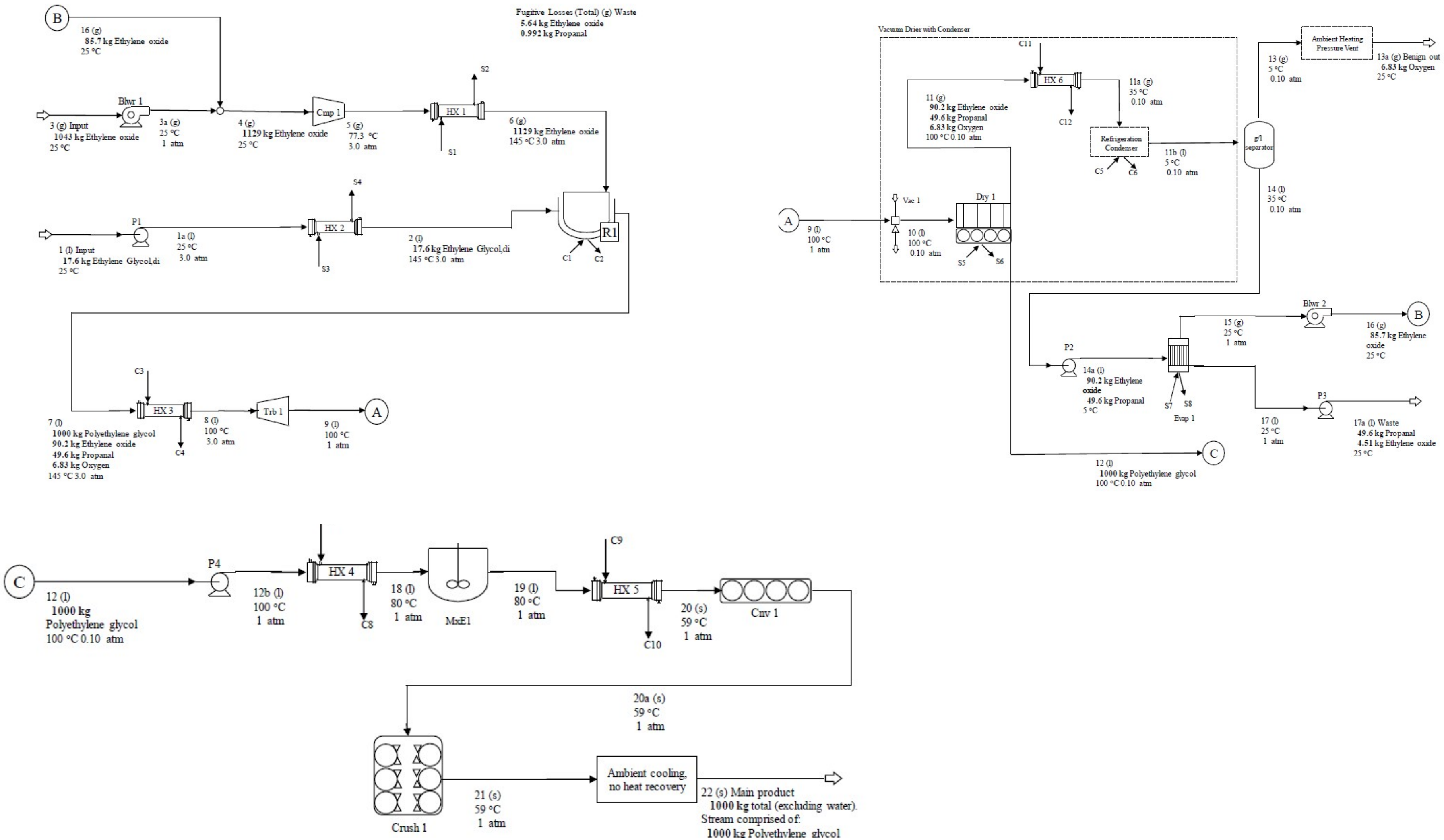

Fig. S 1 Process Diagram of PEG 6000

Table S 1 Progression of HPMC K Grade GTGs and Methodology for Viscosity Reduction

Product	Viscosity (cp)	Methodology that GTG will include
Methocel K300 M	300,000	-K grade synthesis from dissolving pulp, methyl chloride, and propylene oxide
Methocel K100 M	100,000	-Grind Methocel K 300 M (US 4820813)
Methocel K4 M	4,000	-Grind Methocel K 300 M (US 4820813) -Acid catalyzed depolymerization with HCl to get to Methocel K 4 M (US 11407842 B2)
Methocel K100 LV	100	-Grind Methocel K 300 M (US 4820813) -Acid catalyzed depolymerization with HCl to get to Methocel K 100 LV (US 11407842 B2)
Methocel K3 LV	3	-Grind Methocel K 300 M (US 4820813) -Acid catalyzed depolymerization with HCl to get to Methocel K 4 M (US 11407842 B2) -Acid catalyzed depolymerization with HCl and pretreatment with hydrogen peroxide to get to Methocel K 3 LV (WO 2009/061815 A1)

Table S 2 Life Cycle Inventory data of each gtg developed

gtg Inputs per 1000 kg of product	**HPMC K 100 M**	**HPMC K 4 M**	**HPMC K 100 LV**	**HPMC K 3 LV**
HPMC K 300 M (kg)	1000	997	993	989
Hydrogen Chloride (kg)	0	1.3	2.58	3.36
Sodium Bicarbonate (kg)	0	3.73	7.43	9.68
Hydrogen Peroxide (kg)	0	0	0	13.8

Electricity (MJ)	56	97	87	139
Heating Steam (MJ)	0	0.5	1.2	3.6

Table S 3 LCIA data for each gtg input and each Methocel product

	Basis	GWP 100, kg CO_2	Acidification, kg SO_2	Eutrophication, kg N	OzoneDepletion, kg CFC-11	Smog, kg O_3	Blue water, kg H_2O
Hydrogen chloride	1 kg	1.28	8.2E-03	1.7E-04	9.4E-09	0.26	4.09
Sodium bicarbonate	1 kg	1.21	1.2E-02	2.2E-03	2.6E-09	0.14	2.48
hydrogen peroxide	1 kg	1.90	8.8E-03	1.5E-04	1.6E-09	0.14	2.51
Electricity	1 MJ	.16	3.4E-04	1.8E-05	2.4E-09	0.01	0.58
Steam	1 MJ	.09	5.1E-04	7.6E-06	4.4E-12	0.00	0.12
HPMC K 300 M	1000 kg	3,539	17.9	.95	1.16E-01	487	12,617
HPMC K 100 M	1000 kg	3,547	17.9	.96	1.16E-01	488	12,650
HPMC K 4 M	1000 kg	3,550	17.9	.96	1.16E-01	487	12,645
HPMC K 100 LV	1000 kg	3,544	17.9	.97	1.15E-01	486	12,611

HPMC K 3 LV	1000 kg	3,570	18.0	.97	1.15E-01	487	12,635

Table S 4 LCIA values of all analyzed excipients

	NREc (includes NRE electric) MJ HVV	**NREt = NREc + NREm MJ HVV**	**GWP 100. kg CO_2**	**Acidification. kg SO_2**	**Eutrophication. kg N**	**Ozone Depletion. kg CFC-11**	**Smog. kg O_3**	**Blue water kg H_2O**
HPMC E grade	60126.89	82575.26	2890.30	21.26	0.93	0.22	525.80	9537.77
hydroxypropyl cellulose	87135.62	127837.62	4815.93	28.01	1.02	0.00	2158.66	14643.66
methyl cellulose	57107.05	77409.16	2609.64	20.39	0.94	0.18	353.64	8924.60
HEC 2p5 MS	67354.48	96523.57	3696.63	23.65	1.00	0.00	387.60	10331.08
Polysorbate 80. Tween 80	16871.31	41229.82	845.93	9.67	3.53	0.00	194.11	16293.40
PVP	95593.56	187230.36	6576.37	48.03	57.78	0.00	376.91	20131.12
microcrystalline cellulose	82124.87	105009.46	3595.91	34.36	1.36	0.00	613.43	11096.93
ethyl cellulose 2p4 DS	67619.33	96423.82	3455.32	32.33	0.90	0.00	573.83	10699.88
carboxymethylcellulose	92089.29	111867.69	5165.94	35.74	2.49	0.00	632.44	17511.57
HPMCAS	165085.79	230006.42	10407.49	66.49	2.08	0.10	937.09	35138.67
Copovidone	107562.71	185371.86	7252.94	46.90	36.85	0.00	730.56	20744.56
Polyethylene glycol	17880.19	54923.63	1481.05	6.40	0.18	0.00	232.94	5608.83
Polyvinyl alcohol	50702.07	90642.64	3332.77	23.75	0.55	0.00	615.39	8246.61
MAA-co-EA	36855.01	63002.66	1969.12	23.89	4.84	0.00	490.06	44510.27
HPMC K100M	54628.57	71603.08	2386.60	17.87	0.96	0.12	487.66	8429.91
HPMC K4M	54633.94	71595.53	2392.96	17.89	0.96	0.12	487.21	8439.83
HPMC K100 LV	54506.14	71455.90	2391.16	17.88	0.97	0.12	486.40	8420.09
HPMC K3 LV	54801.47	71859.00	2421.34	17.99	0.97	0.11	487.43	8461.05

crosslinked CMC	95719.80	117340.96	5424.06	37.67	2.67	0.00	661.44	18101.36
eudragit E PO	24704.35	60658.36	1814.80	25.00	6.50	0.00	418.65	4617.42
starch 1500	7909.34	8621.80	-894.83	7.71	0.82	0.00	53.74	88488.43
alpha lactose monohydrate	71596.42	86842.86	7358.20	72.80	8.00	0.00	519.50	1466520.01
sorbitol excipient	19680.28	21739.18	29.47	12.19	0.93	0.00	133.35	86606.49
glycerol	3519.73	3519.73	231.24	1.41	0.04	0.00	25.34	447.33
mannitol	19409.84	21539.19	-39.39	12.32	0.95	0.00	133.63	89415.07
magnesium stearate	14192.86	16396.18	-174.78	16.88	13.73	0.00	119.09	2671.65
tartaric acid	39325.30	51622.76	2699.81	31.78	0.47	0.00	256.75	3642.21
crospovidone	104099.54	206627.86	7230.84	52.12	63.07	0.00	420.59	22429.49
dextrose	15543.16	16244.04	-354.09	10.14	0.85	0.00	77.61	88193.36
sodium starch glycolate	43085.73	53418.07	1225.94	28.39	2.97	0.00	431.17	202967.47
Sodium lauryl sulfate (SLS)	38339.86	76734.17	2454.01	23.56	0.35	0.00	404.23	7367.97
sodium stearyl fumarate	19286.79	40377.32	844.03	16.61	12.43	0.00	210.54	4502.26
citric acid	9763.57	21829.43	-443.67	23.35	4.24	0.00	289.07	398750.37
sucrose	6879.66	7848.66	-990.78	7.41	5.73	0.00	187.94	384001.35
sucralose	207234.19	240412.61	12604.98	88.37	12.06	0.00	2369.97	697918.24
L-arginine	46990.08	67280.53	1360.82	47.77	4.99	0.00	394.45	121616.17
Excipient Average	55832.19	82100.59	3001.89	28.00	7.20	0.03	496.62	109872.96

Table S 5 Normalized LCIA values of all analyzed excipients

	NREc (includes NRE electric)	**NREt = NREc + NREm**	**GWP 100**	**Acidification**	**Eutrophication**	**Ozone Depletion**	**Smog**	**Blue water**
HPMC E grade	1.1	1.0	1.0	0.8	0.1	8.1	1.1	0.1
hydroxypropyl cellulose	1.6	1.6	1.6	1.0	0.1	0.0	4.3	0.1
methyl cellulose	1.0	0.9	0.9	0.7	0.1	6.8	0.7	0.1
HEC 2p5 MS	1.2	1.2	1.2	0.8	0.1	0.0	0.8	0.1
Polysorbate 80. Tween 80	0.3	0.5	0.3	0.3	0.5	0.0	0.4	0.1
PVP	1.7	2.3	2.2	1.7	8.0	0.0	0.8	0.2

microcrystalline cellulose	1.5	1.3	1.2	1.2	0.2	0.0	1.2	0.1
ethyl cellulose 2p4 DS	1.2	1.2	1.2	1.2	0.1	0.0	1.2	0.1
carboxymethylcellulose	1.6	1.4	1.7	1.3	0.3	0.0	1.3	0.2
HPMCAS	3.0	2.8	3.5	2.4	0.3	3.8	1.9	0.3
Copovidone	1.9	2.3	2.4	1.7	5.1	0.0	1.5	0.2
Polyethylene glycol	0.3	0.7	0.5	0.2	0.0	0.0	0.5	0.1
Polyvinyl alcohol	0.9	1.1	1.1	0.8	0.1	0.0	1.2	0.1
MAA-co-EA	0.7	0.8	0.7	0.9	0.7	0.0	1.0	0.4
HPMC K100M	1.0	0.9	0.8	0.6	0.1	4.3	1.0	0.1
HPMC K4M	1.0	0.9	0.8	0.6	0.1	4.3	1.0	0.1
HPMC K100 LV	1.0	0.9	0.8	0.6	0.1	4.3	1.0	0.1
HPMC K3 LV	1.0	0.9	0.8	0.6	0.1	4.3	1.0	0.1
crosslinked CMC	1.7	1.4	1.8	1.3	0.4	0.0	1.3	0.2
eudragit E PO	0.4	0.7	0.6	0.9	0.9	0.0	0.8	0.0
starch 1500	0.1	0.1	-0.3	0.3	0.1	0.0	0.1	0.8
alpha lactose monohydrate	1.3	1.1	2.5	2.6	1.1	0.0	1.0	13.3
sorbitol excipient	0.4	0.3	0.0	0.4	0.1	0.0	0.3	0.8
glycerol	0.1	0.0	0.1	0.1	0.0	0.0	0.1	0.0
mannitol	0.3	0.3	0.0	0.4	0.1	0.0	0.3	0.8
magnesium stearate	0.3	0.2	-0.1	0.6	1.9	0.0	0.2	0.0
tartaric acid	0.7	0.6	0.9	1.1	0.1	0.0	0.5	0.0
crospovidone	1.9	2.5	2.4	1.9	8.8	0.0	0.8	0.2
dextrose	0.3	0.2	-0.1	0.4	0.1	0.0	0.2	0.8
sodium starch glycolate	0.8	0.7	0.4	1.0	0.4	0.0	0.9	1.8
Sodium lauryl sulfate (SLS)	0.7	0.9	0.8	0.8	0.0	0.0	0.8	0.1
sodium stearyl fumarate	0.3	0.5	0.3	0.6	1.7	0.0	0.4	0.0
citric acid	0.2	0.3	-0.1	0.8	0.6	0.0	0.6	3.6
sucrose	0.1	0.1	-0.3	0.3	0.8	0.0	0.4	3.5
sucralose	3.7	2.9	4.2	3.2	1.7	0.0	4.8	6.4
L-arginine	0.8	0.8	0.5	1.7	0.7	0.0	0.8	1.1

Table S 6 Comparison of Total Energy and Process Impacts of Pharmaceutical Excipients

	Total impact	**Energy impact**	**Process impact**	**Process / Total this category**
Global warming potential, kg CO_2				
PVP	6576.37	4464.19	2112.18	0.32
Crospovidone	7230.84	4870.25	2360.59	0.32
Copovidone	7252.94	5769.35	1483.59	0.20
PEG	1481.05	955.87	525.17	0.35
Polysorbat 80	1624.73	962.15	662.58	0.41
PVA	3332.77	2991.83	340.94	0.10
Maize starch	-895	458.39	-1353.2	0.15
HPMCAS	10.407	10.341	66	0.10
Eudragit EPO	1814.80	1436.86	377.94	0.21
Eudragit L 100-55	2576.63	2321.97	254.66	0.10
Mannitol	-39	1214.75	-1254	0.12
Sorbitol	29	1242.11	-1213	0.12
Magnesium stearate	-175	912.90	-1.088	0.60
Lactose	7.358	4506.46	2.852	0.51
Sodium stearyl fumarate	844	1.233	-389	0.60
Sucralose	1.26E+04	1.32E+04	-617	0.27
Citric acid	-444	583	-1.027	0.80
Sucrose	-991	394	-1.384	0.82
Ozone depletion, kg CFC-11				

MC	0.18	0.00	0.18	1.00
HPMC K grade	0.12	0.00	0.12	1.00
HPMC E grade	0.22	0.00	0.22	1.00
HPMCAS	0.10	0.00	0.10	1.00
Eutrophication, kg N				
PVP	57.78	0.35	57.43	0.99
Copovidone	36.85	0.53	36.32	0.99
Crospovidone	63.10	0.38	62.69	0.99
Eudragit EPO	6.50	0.24	6.26	0.96
Eudragit L 100-55	4.84	0.30	4.54	0.94
MCC	1.36	0.62	0.74	0.54
CMC linear	2.49	0.68	1.80	0.72
CMC cross-linked	2.67	0.71	1.95	0.73
HPMCAS	2.08	1.08	1.00	0.48
HPMC K grade	0.96	0.42	0.53	0.56
HPMC E grade	0.93	0.45	0.49	0.52
HPC	1.02	0.65	0.37	0.36
EC	0.90	0.52	0.38	0.43
HEC	1.00	0.47	0.52	0.52
MC	0.94	0.43	0.52	0.55
Maize starch	0.82	0.09	0.73	0.90
Sodium Strach glycolate	2.97	0.49	2.48	0.84
Mannitol	0.95	0.23	0.73	0.76
Sorbitol	0.93	0.23	0.70	0.76
Magnesium stearate	13.70	0.17	13.60	0.99
Tartaric acid	0.47	0.39	0.08	0.16
Lactose	8.00	0.79	7.21	0.90
Glucose	0.85	0.13	0.72	0.85
Sodium stearyl fumarate	12.4	0.19	12.2	0.99
Sucralose	12.1	1.66	10.4	0.86
Arginine	4.99	0.50	4.49	0.90
Citric acid	4.24	0.27	3.97	0.94
Sucrose	5.73	0.15	5.60	0.98
Smog, kg O_3				

PVP	376.91	155.53	221.38	0.59
Copovidone	730.56	255.74	474.82	0.65
Crospovidone	420.59	173.01	247.58	0.59
Eudragit EPO	418.65	133.53	285.12	0.68
Eudragit L 100-55	490.06	165.24	324.82	0.66
PVA	615	165	450	0,73
MCC	613.43	329.29	284.14	0.46
CMC linear	632.44	368.62	263.82	0.42
CMC cross-linked	661.44	384.63	276.81	0.42
EC	573.83	275.21	298.62	0.52
HEC	387.60	254.27	133.34	0.34
MC	353.64	221.86	131.78	0.37
HPMC K grade	487.70	220.31	267.39	0.55
HPMC E grade	525.80	233.10	292.72	0.56
HPMCAS	937.09	578.80	358.29	0.38
HPC	2158.69	343.48	1815.22	0.84
Magnesium stearate	119.10	92.10	27.03	0.23
Tartaric acid	256.75	225.35	31.40	0.12
Lactose	519.50	429.71	89.80	0.17
Sodium stearyl fumarate	211	99.8	111	0.53
Sodium lauryl sulfate	404	164	240	0.59
Sucralose	2.370	857	1.513	0.64
Arginine	394	272	123	0.31
Citric acid	289	144	145	0.50
Sucrose	188	77.3	111	0.59
Acidification, kg SO_2				
MC	20.39	15.37	5.03	0.25
HPMC K grade	17.87	13.98	3.89	0.22
HPMC E grade	21.26	16.50	4.77	0.22
HPMCAS	66.49	54.24	12.24	0.18
EC	32.33	19.86	12.46	0.39
HEC	23.65	20.42	3.22	0.14
CMC linear	35.74	27.57	8.16	0.23
CMC cross-linked	37.67	28.79	8.87	0.24

MCC	34.36	22.47	11.89	0.35
Maize starch	7.71	3.55	4.16	0.54
Sodium starch glycolate	28.4	15.43	13.00	0.46
Eudragit EPO	25.00	10.21	14.79	0.59
Eudragit L 100-55	23.89	14.20	9.69	0.41
PVP	48.03	39.25	8.78	0.18
Copovidone	46.90	38.93	7.97	0.17
Crospovidone	52.12	42.32	9.79	0.19
Mannitol	12.32	8.15	4.17	0.34
Sorbitol	12.19	8.16	4.03	0.33
Magnesium stearate	16.90	5.08	11.80	0.70
Tartaric acid	31.80	16.72	15.10	0.47
Lactose	72.80	23.27	49.53	0.68
Glucose	10.14	6.05	4.09	0.40
Sodium stearyl fumarate	16.6	5.75	10.9	0.65
Sodium lauryl sulfate	23.6	12.8	10.8	0.46
Sucralose	88.4	60.8	27.6	0.31
Arginine	47.8	15.7	32.1	0.67
Citric acid	23.4	3.27	20.1	0.86
Sucrose	7.41	2.11	5.29	0.72

Table S 7 Gate-to-Gate Contributions to Process Emissions in Excipient Manufacturing

Excipient	GWP	Acidification	Eutrophication	Ozone Depletion	Smog
MCC	Biogenic CO2 credit of -1602 kg/1000 kg. Due to tree growth for cellulose.	9.5 kg SO_2 eq / 1000 kg. Emissions primarily (80 %) from HCl emissions to air during hydrolytic degradation process (strong mineral acid use) and the HCl CTG.	0.74 kg Neq / 1000 kg. Emissions from liquid ammonium. Most of these are from N fertilizer for growing biomass for cellulose production.	n.a.	The process emission impact is 284 kg O_3eq / 1000 kg. 56% of these emissions primarily from fugitive chlorine gas emissions during chlorine and hydrogen chloride production.
HPMC K	Biogenic CO2 credit of -1161 kg/1000 kg. Due	3.9 kg SO_2 eq / 1000 kg. Emissions primarily	0.53 kg Neq / 1000 kg. Emissions from liquid	0.116 kg CFC-11eq / 1000 kg. Emissions due	The process emission impact is 267 kg O_3eq /

	to tree growth for cellulose.	from ammonia, hydrogen chloride (HCl) and sulfur oxides (SOx). 41% of the process emissions impact is from cellulose CTG (SOx) (and 58% is from methyl chloride (mostly HCl emissions).	ammonium. Most of these are from N fertilizer for growing biomass for cellulose production.	to methyl chloride used in production.	1000 kg. 80% of impact due to chlorine gas emissions. These are primarily from fugitive chlorine gas emissions during chlorine and hypochlorous acid production in propylene oxide CTG.
HPMC E	Biogenic CO2 credit of -1051 kg/1000 kg. Due to tree growth for cellulose.	4.77 kg SO_2 eq / 1000 kg. Emissions primarily from hydrogen chloride (HCl), sulfur oxides (SOx), and nitrogen oxides (NOx). About 70% from methyl chloride CTG (mostly HCl) and the rest Is from the cellulose CTG (mostly SOx)	0.486 kg Neq / 1000 kg. Emissions from liquid ammonium. Most of these are from N fertilizer for growing biomass for cellulose production.	0.215 kg CFC-11eq / 1000 kg. Emissions due to methyl chloride used in production.	The process emission impact is 293 kg O_3eq / 1000 kg. Emissions primarily from fugitive chlorine gas emissions during chlorine and hypochlorous acid production in propylene oxide CTG.
HPC	Biogenic CO2 credit of -750 kg/1000 kg. Due to tree growth for cellulose.	n.a.	0.370 kg Neq / 1000 kg. Emissions from liquid ammonium. Most of these are from N fertilizer for growing biomass for cellulose production.	n.a.	The process emission impact is 1815 kg O_3eq / 1000 kg. Emissions primarily from fugitive chlorine gas emissions during chlorine and hypochlorous acid production in propylene oxide CTG.
HEC	Biogenic CO2 credit of -907 kg/1000 kg. Due to	3.22 kg SO_2 eq / 1000 kg. Emissions primarily	0.523 kg Neq / 1000 kg. Emissions from liquid	n.a.	The process emission impact is 133 kg O_3eq /

	tree growth for cellulose.	from ammonia, SOx, and NOx. Most of the ammonia emissions are from CO2 production in the CO supply chain. The SOx emissions are mostly from the cellulose supply chain.	ammonium. Most of these are from N fertilizer for growing biomass for cellulose production.		1000 kg. Mainly driven by organic fugitive emissions from the supply chain. About half of these are from the ethylene oxide supply chain and 20% are from tert-butanol CTG. The ethylene oxide CTG process smog emissions are mostly from the refinery (naphtha, propylene, ethylene, pyrolysis gas).
MC	Biogenic CO2 credit of -1119 kg/1000 kg. Due to tree growth for cellulose.	5.03 kg SO_2 eq / 1000 kg. Emissions primarily from ammonia, hydrogen chloride (HCl), sulfur oxides (SOx), and nitrogen oxides (NOx). 70% of process emissions impact are from methyl chloride CTG, mostly HCl emissions in the GTG and in the HCl portion of the supply chain.	0.517 kg Neq / 1000 kg. Emissions from liquid ammonium. Most of these are from N fertilizer for growing biomass for cellulose production.	0.183 kg CFC-11eq / 1000 kg. Emissions due to methyl chloride used in production.	The process emission impact is 132 kg O_3eq / 1000 kg. Emissions primarily from fugitive chlorine gas emissions during chlorine, hydrogen chloride, and sodium hydroxide production.

HPMCAS	1174 kg CO_2eq from process emissions / 1000 kg. 51 % is from CO_2 and 42 % of this is methane. 48% of this is from the butanedioic anhydride CTG (21% CH4 and 79% CO2), and 19% is from sodium acetate CTG (73% CH4). Methane emissions are from natural gas extraction. Biogenic CO2 credit of -1108 kg/1000 kg. Due to tree growth for cellulose.	12.2 kg SO_2 eq / 1000 kg. Emissions primarily from ammonia, hydrogen chloride (HCl), sulfur oxides (SOx), and nitrogen oxides (NOx). About 27% is from the hydroxypropyl methyl cellulose CTG (mostly HCl and SOx) and 32% is from the sodium acetate CTG (mostly ammonia to air), and 20% is from the acetic anhydride CTG (mostly ammonia to air and NOx).	1.0 kg Neq / 1000 kg. Emissions from liquid ammonium. Most of these are from N fertilizer for growing biomass for cellulose production. Ammonia emissions to air from Succinic anhydride ctg.	0.101 kg CFC-11eq / 1000 kg. Emissions due to methyl chloride used in production.	The process emission impact is 358 kg O_3eq / 1000 kg. About half of impact is fugitive chlorine gas emissions during hypochlorous acid production. The other contributing chemicals are Nox, acetic acid, refinery emissions, and methanol.
EC	Biogenic CO2 credit of -849 kg/1000 kg. Due to tree growth for cellulose.	12.5 kg SO_2 eq / 1000 kg. Emissions primarily from HCl during chloroethane production. Cellulose has some SOx and Nox emissions. These may have actually been operation of machinery that were not counted as energy. The process impact of cellulose production is 2.13 kg SO2 / 1000 kg of cellulose, and there is	0.384 kg Neq / 1000 kg. Emissions from liquid ammonium. Most of these are from N fertilizer for growing biomass for cellulose production.	n.a.	The process emission impact is 299 kg O_3eq / 1000 kg. Chlorine emissions from chloroethane ctg are 26% of impact. Toluene emissions are 28% of impact. Rest is mostly other organic emissions.

		0.557 kg of cellulose in this CTG. So, the impact from cellulose CTG process emissions is 1.19 kg SO2eq. This is about 10% of the process emissions in this CTG.			
CMC linear	Biogenic CO2 credit of -1209 kg/1000 kg. Due to tree growth for cellulose and corn growth.	8.16 kg SO_2 eq / 1000 kg. Half of this is from ammonia emissions to air. Most of these are from growing biomass for cellulose production. The rest of the emissions are from SOx and Nox.	1.8 kg Neq / 1000 kg. Over ¾ is from liquid ammonia and ammonium emissions to air. Ammonium emissions from cellulose CTG and sodium carbonate GTG. Ammonia air emissions are from CO and CO2 production.	n.a.	The process emission impact is 264 kg O_3eq / 1000 kg. 30 % of this is from chlorine emissions to air. 23 % is from propylene emissions to air. The rest are mostly other organics. 3.6% is from cellulose CTG.
CMC cross-linked	Biogenic CO2 credit of -1225 kg/1000 kg. Due to tree growth for cellulose and corn growth.	8.9 kg SO_2 eq / 1000 kg. Half of this is from ammonia emissions to air. Most of these are from growing biomass for cellulose production. 74 % of the 8.9 kg SO_2eq / 1000 kg crosslinked CMC impact is from the sodium chloroacetate CTG.	1.95 kg Neq / 1000 kg. Process emissions account for 1.95 kg Neq / 1000 kg crosslinked CMC. Over ¾ of this is from ammonia emissions as liquid. 0.5 kg Neq is from cellulose CTG. 71 % of the 1.95 kg Neq / 1000 kg crosslinked CMC is from sodium chloroacetate CTG.	n.a.	The process emission impact is 277 kg O_3eq / 1000 kg. 30 % of this is from chlorine emissions to air. 22 % is from propylene emissions to air. The rest are mostly other organics. 3.5% is from the cellulose CTG.

PVP	2112 kg CO_2eq from process emissions / 1000 kg. CO_2 and CH_4 emissions are both significant, as CO_2 is 59 % of the process emissions, and CH_4 is most of the rest. Most of the CO_2 process emissions are from acetylene production in the NVP supply chain. Methane emissions come mostly from acetylene and 2-pyrrolidone manufacturing.	8.78 kg SO_2 eq / 1000 kg. 55 % of this is from ammonia with the remainder from NO_x and SO_x emissions. The ammonia emissions are from 2-pyrrolidone and ammonia GTGs.	8.33 kg Neq / 1000 kg. 95 % of the eutrophication impact is from process ammonia emissions, which are all from 2-pyrrolidone.	n.a.	The process emission impact is 221 kg O_3eq / 1000 kg. Half of these are formaldehyde emissions to air in the 1,4-butanediol supply chain. Most of these are from formaldehyde production.
Copovidone	1484 kg CO_2eq from process emissions / 1000 kg. CO_2 and CH_4 emissions are both significant, as CO_2 is 57 % of the process emissions, and CH_4 is most of the rest. Most of the CO_2 process emissions are from acetylene production in the NVP supply chain. Methane emissions come mostly from acetylene and 2-	7.97 kg SO_2 eq / 1000 kg. 54 % of this is from ammonia with the remainder from NO_x and SO_x emissions. The ammonia emissions are from 2-pyrrolidone and ammonia GTGs.	4.9 kg Neq / 1000 kg. Over 92 % of the eutrophication impact is from process liquid ammonia emissions, which are all from 2-pyrrolidone.	n.a.	The process emission impact is 475 kg O_3eq / 1000 kg. 16% of these are formaldehyde emissions to air in the 1,4-butanediol supply chain, and most of these are from formaldehyde production. The remainder is a mix of ethylene, propylene, vinyl acetate, Nox, acetic acid, naphtha, and other organics.

	pyrrolidone manufacturing.				
Crospovidone	2361 kg CO_2eq from process emissions / 1000 kg crospovidone. CO_2 and CH_4 emissions are both significant, as CO_2 is 59 % of the process emissions, and CH_4 is most of the rest. Most of the CO_2 process emissions are from acetylene production in the NVP supply chain. Methane emissions come mostly from acetylene and 2-pyrrolidone manufacturing.	9.79 kg SO_2 eq / 1000 kg crospovidone. Process emissions account for 20 % of the total impact, half of this is from ammonia with the remainder from NO_x and SO_x emissions. The ammonia emissions are from 2-pyrrolidone and ammonia GTGs.	8.6 kg Neq / 1000 kg crospovidone. 94 % of the eutrophication impact is from process liquid ammonia emissions, which are all from 2-pyrrolidone.	n.a.	The process emission impact is 248 kg O_3eq / 1000 kg crospovidone. About 59 % of total emissions are process emissions. Half of these are formaldehyde emissions to air in the 1,4-butanediol supply chain. Most of these are from formaldehyde production.
PVA PVA	341 kg CO_2eq from process emissions / 1000 kg. 77 % from methane emissions. Nearly all of CH4 emissions are from natural gas extraction. 60% of the impact is from the vinyl acetate CTG and 25% is from the methanol CTG.	4.40 kg SO_2 eq / 1000 kg. 65% is from ammonia to air from the CO and CO2 gtgs. The remainder is a mix of Nox and SOx.	0.242 kg Neq / 1000 kg Mostly ammonia to air from CO and CO2 gtgs.	n.a.	The process emission impact is 450 kg O_3eq / 1000 kg. 36% from vinyl acetate emissions to air (PVA and vinyl acetate gtgs), 34% from ethylene emissions (mostly vinyl acetate gtg). Rest is mix of other organic fugitive emissions from the supply chain.

PEG 6000	525 kg CO_2eq from process emissions / 1000 kg. Emissions from GTG production of ethylene oxide from ethylene and oxygen.	n.a.	n.a.	n.a.	The process emission impact is 144 kg O_3eq / 1000 kg. Most of the emissions are organics from the refinery including naphtha, ethylene, propylene, and pyrolysis gas. The ethylene oxide CTG is responsible for 74% of the process emission smog impact.
Polysorbate 80	663 kg CO_2eq from process emissions / 1000 kg. 40 % is from CO_2 and 58 % of this is methane. Emissions from sorbitan monooleate CTG (mainly methane emissions from anaerobic activity in palm oil mill effluent). Additional CH4 emissions are from ethylene oxide GTG. Most CO2 emissions are from the ethylene oxide GTG. Biogenic CO2 credit of -779 kg/1000 kg. Due to palm fruit and corn growth.	3.39 kg SO_2 eq / 1000 kg. 80% of the emissions are from ammonia emissions to air. 72% of this is from palm oil production and 16% from corn production. The rest is mainly Sulfur dioxide and NO_x. Nox and SOx emissions from a mix of gtgs including sulfuric acid production and palm fruit production.	3.34 kg Neq / 1000 kg. Mainly due to liquid nitrate emissions to soil during palm fruit production.	n.a.	The process emission impact is 93.6 kg O_3eq / 1000 kg. This is nearly all due to organic emissions near the refinery (naphtha, ethylene, propylene, and pyrolysis gas).

Eudragit EPO	The impact from process emissions is 378 kg CO_2eq / 1000 kg Eudragit E PO. Of this, 205 kg is from CO_2 and 173 kg is from methane. 87 % of these emissions are from the butyl methacrylate and dimethylaminoethyl methacrylate supply chains.	The impact from process emissions is 14.8 kg SO_2eq / 1000 kg Eudragit E PO. Of this, the majority is from SO_x and ammonia emissions to air. 79 % of these emissions are from the butyl methacrylate and dimethylaminoethyl methacrylate supply chains.	The impact from process emissions is 6.26 kg Neq / 1000 kg Eudragit E PO. Most of these emissions come from liquid ammonia, with 73 % originating from the butyl methacrylate and dimethylaminoethyl methacrylate supply chains.	n.a.	The impact from process emissions is 285 kg O_3eq / 1000 kg Eudragit E PO. These originate from a combination of organic emissions within the supply chain. 43% of the impact is from methyl methacrylate emissions. Much of the rest of the impact is from the refinery and nearby processes and these include propylene, naphthta, ethylene, Nox, etc. 51% of the total process emissions impact is from the dimethylaminoethyl methacrylate CTG and 20% is from butyl methacrylate CTG.
Eudragit L100-55	The impact from process emissions is 255 kg CO_2eq / 1000 kg Eudragit L100-55. Of this, 160 kg is from CO_2, 65 kg from methane, and 30 kg from N_2O. Emissions primarily from methacrylic acid supply chain. Biogenic CO2 credit of -608 kg/1000	Emissions primarily from sulfur oxides (SOx) (60%) and ammonia (33%). Ammonia emissions were from corn production, ammonia production, and the methacrylic acid gtg. SOx emissions are primarily from the sulfuric acid CTG.	Emissions primarily from ammonia in the methacrylic acid supply chain.		Mainly driven by organic fugitive emissions from the supply chain. 15% is from acrolein emissions, 14% is from ethanol emissions, and much of the rest is from propylene, ethylene, naphtha, and pyrolysis gas. These emissions are from the refinery

	kg. Due to palm fruit and corn growth.				and other gtgs near the refinery.
Maize starch	79.8 kg CO_2eq from process emissions / 1000 kg maize starch. Most of this is from nitrous oxide emissions to air, and these are largely from application of N fertilizer to grow corn. Biogenic CO2 credit of -1433 kg/1000 kg. Due to corn growth.	4.16 kg SO_2 eq / 1000 kg maize starch. Most of this is from ammonia emissions to air, and these are largely from application of N fertilizer to grow corn.	0.732 kg Neq / 1000 kg maize starch.	n.a.	n.a.
SSG	Biogenic CO2 credit of -1760 kg/1000 kg. Due to potato and corn growth.	13.0 kg SO_2 eq / 1000 kg SSG. Most (77%) of the process acidification emissions are ammonia to air. About 70 % of this is from potato starch CTG, and most of the rest is from the sodium chloroacetate CTG.	2.48 kg Neq / 1000 kg SSG. Process eutrophication emissions are a mix of nitrate (l), ammonia (a), ammonia (l), and phosphates (l). About 70% of this is from the potato starch CTG, and the remainder from sodium chloroacetate CTG, of which most is ammonia emissions from the sodium carbonate GTG.	n.a.	The total impact is 163 kg O_3eq / 1000 kg SSG. Ethanol emissions to air make up 50 % of process emissions. These are from the sodium starch glycolate GTG. The rest are mostly from Cl_2, NO_x, NMVOC in the sodium chloroacetate and potato starch CTGs.
Mannitol	167 kg CO_2eq from process emissions / 1000 kg mannitol. 76 kg CO_2eq is from CO_2 and 71 kg CO_2eq of this is	4.17 kg SO_2 eq / 1000 kg mannitol. Of this, 3.59 kg SO_2eq is from ammonia emissions to air, and nearly all of this	0.727 kg Neq / 1000 kg mannitol). Of this, 4.89 kg Neq is from phosphate emissions to liquid (soil) and 0.227	n.a.	n.a.

	from N_2O. Nearly all the N_2O emission (69 kg) is from corn production, which has 3.5 kg CO_2 process emissions and 66.2 kg CO_2eq from N_2O process emissions per 1000 kg. Biogenic CO2 credit of -1421 kg/1000 kg. Due to corn growth.	is from corn production.	kg is from ammonia air emissions. The process impact from corn growth is 0.674 kg Neq / 1000 kg corn.		
Lactose	4619 kg CO_2eq / 1000 kg lactose monohydrate are from process emissions. 3703 kg CO_2eq of this are from methane emissions to air and 828 are from nitrous oxide emissions to air. These emissions are mostly from milk production. Biogenic CO2 credit of -1767 kg/1000 kg. Due to corn, soybean, and cotton growth.	49.5 kg SO_2 eq / 1000 kg lactose. Of this, 37.6 kg SO_2eq is from ammonia, and the rest is from SO_x and NO_x. The milk CTG is responsible for all 49.5 kg SO_2eq of the process emissions.	7.21 kg Neq / 1000 kg lactose. Of this, 4.66 is from phosphate liquid emissions and 2.4 kg is from ammonia emissions to air. Nearly all the process emission impact is from the milk CTG.	n.a.	The total impact is 89.8 kg O_3eq / 1000 kg lactose. Of this, 76 % is from NO_x emissions. 90 % of the smog forming process emissions are from the milk ctg. Corn production produces 3.62 kg O_3eq / 1000 kg corn, and 10,255 kg of corn are used / 1000 kg lactose monohydrate. Thus, 37 kg O_3eq / 1000 kg of lactose monohydrate is from corn that is fed to the cows.
Sorbitol	162 kg CO_2eq from process emissions / 1000 kg sorbitol. 74 kg CO_2eq of this is from CO_2 and 69 kg CO_2eq of this is from N_2O.	4.03 kg SO_2 eq / 1000 kg sorbitol. Of this, 3.48 kg SO_2eq is from ammonia emissions to air, and nearly all of this is from corn production.	0.703 kg Neq / 1000 kg sorbitol. Of this, 4.73 kg Neq is from phosphate emissions to liquid (soil) and 0.219 kg is from ammonia air	n.a.	n.a.

	Nearly all the N_2O emission (69 kg) is from corn production, which has 3.5 kg CO_2 process emissions and 66.2 kg CO_2eq from N_2O process emissions per 1000 kg. Biogenic CO2 credit of -1374 kg/1000 kg. Due to corn growth.		emissions due to corn growth.		
MgSt	The process emission impact is 1362 kg CO_2eq / 1000 kg magnesium stearate. Most (1229 kg CO_2eq) of the process GWP emissions are from methane emissions to air. These emissions are mostly from the crude palm oil GTG. The large CH_4 emissions from palm oil production is due to anaerobic decomposition of palm oil mill effluent (POME). Biogenic CO2 credit of -2449 kg/1000 kg. Due to palm fruit growth.	The process emission impact is 11.8 kg SO_2eq / 1000 kg magnesium stearate. The process emission impact is dominated by ammonia emissions to air, which result in 9.55 kg SO2eq / 1000 kg magnesium stearate (about 81% of the total process emissions). Most from Palm oil fruit production (at field). Additional ammonia emissions to air are from production of crude palm oil from the fruit bunches.	The process emission impact is 13.6 kg N / 1000 kg magnesium stearate. These emissions are mostly from growing the fruit bunches	n.a.	The process emission impact is 27 kg O_3eq / 1000 kg magnesium stearate. This is due mostly to NO_x emissions. On a 1000 kg magnesium stearate basis, MgOH CTG has 3.2 kg O_3eq, the palm fruit bunch growth gtg has 15 kg O_3eq, N fertilizer has 5.5 kg O_3eq, and P fertilizer has 2.5 kg O_3eq.
SSF	The impact from process emissions is 1821 kg CO_2eq / 1000.	The process emission impact is 10.9 kg SO_2eq / 1000 kg SSF. The	The process emission impact is 12.2 kg N / 1000 kg SSF. Mostly	n.a.	The process emission impact is 111 kg O_3eq / 1000 kg SSF. Of this,

	About 70% of the process emissions are from the octodecanol tree and 32% are from maleic anhydride. Octodecanol is made from palm oil, and crude palm oil refining has a large methane emission from the palm oil effluent stream. Biogenic CO2 credit of -2211 kg/1000 kg. Due to palm fruit growth.	process emissions acidification impact is dominated by ammonia emissions to air (78% of total process emissions). This is primarily from the growth of palm fruit bunches.	from nitrate emissions to soil, which are nearly all from the fresh palm fruit bunches GTG.		65 % is from the SSF GTG, and 20 % is from the octadecanol CTG. Most of the SSFsmog related emissions are toluene emissions to the air.
SLS	n.a.	A total of 208 kg SO_2eq / 1000 kg SLS. Of this, 80% are from the chlorosulfonic acid CTG, and most of these are from SO_x emissions in the supply chain.	n.a.	n.a.	The process emission impact is 240 kg O_3eq / 1000 kg SLS. Of this, 74 % are from the dodecanol CTG and 17 % are from chlorosulfonic acid GTG. Most of these are alkenes and naphtha from refinery emissions.
Tartaric acid	n.a.	A total of 15.1 kg SO_2eq / 1000 kg tartaric acid is from process emissions, and 14.0 kg SO_2eq are from SO_x emissions from sulfuric acid production (CTG).	There are 0.0769 kg Neq from process emissions / 1000 kg tartaric acid. Of this, 0.0329 kg Neq are from NO_x emissions and 0.022 kg Neq are from ammonia emissions. Carbon dioxide is in the supply chain of calcium	n.a.	

			hydroxide and is a byproduct of ammonia production. This results in 0.037 kg Neq process emissions per 1000 kg tartaric acid. Sulfuric acid accounts for the other 0.04 kg Neq due to NO_x emissions.		
Arginine	Biogenic CO2 credit of -1559 kg/1000 kg. Due to corn growth.	A total of 32.1 kg SO_2eq / 1000 kg arginine. Most of the acidification impact was from SO_x and ammonia emissions. About 73 % of the process emissions impact is from the ammonium sulfate CTG. This is from ammonia emissions during ammonia production and SO_x emissions during sulfuric acid production. The remainder is mostly from dextrose, which is made from corn starch. The dextrose emissions are mainly from ammonia emissions from the field during corn growth.	There are 4.49 kg Neq from process emissions / 1000 kg arginine. Ammonia emissions to liquid and gas phases account for 66 % and 16 % of these emissions. Liquid phosphate emissions account for 14 %. Of the total eutrophication impact, 79 % is from ammonium sulfate production, and 21 % is from dextrose production, mostly (95%) from corn growth.	n.a.	The process emission impact is 123 kg O_3eq / 1000 kg arginine. A large portion (about 40 %) of this is from chlorine emissions. Most of the rest are a mix of NO_x and NMVOC. Of the total process emissions, about 41 % are from the ammonium sulfate CTG, 24 % is from hydrogen chloride CTG, and 26 % is from the sodium hydroxide CTG.
Citric acid	The impact from	A total of 20.1 kg	The process emission	n.a.	The process emission

	process emissions is 2271 kg CO_2eq / 1000. Of this, 94 % is CO2 emissions to air from the sugarcane refining to molasses when bagasse is used for fuel. This portion is mostly offset by biogenic emissions sequestration when the bagasse is grown. Biogenic CO2 credit of -3298 kg/1000 kg. Due to sugarcane growth. Some of this is offset by bagasse combustion emissions.	SO_2eq / 1000 kg citric acid. More than half of this is from SO_x emissions to air, and the rest is from NO_x and ammonia emissions to air. Citric acid production uses a large amount of sulfuric acid, and over half of the acidification process emissions (54 % of the impact) is from sulfuric acid production. About 27 % of the process acidification impact is from molasses CTG, mostly from NOx emissions in the supply chain.	impact is 3.97 kg N / 1000 kg citric acid. 81 % of the process emissions impact is from phosphates released to soil. Most of the process emissions impact is from sugarcane production in the supply chain of molasses. The molasses CTG accounts for 96 % of the process emissions eutrophication impact.		impact is 145 kg O_3eq / 1000 kg citric acid. Most of this is from NO_x emissions, and these are primarily from the molasses CTG (79 % of total process emission impact).
Glucose	Biogenic CO2 credit of -1409 kg/1000 kg. Due to corn growth.	A total of 4.09 kg SO_2eq / 1000 kg glucose. Most (87%) of the process acidification impact is from ammonia emissions to air. Most of these are from corn production, mostly from emissions after application of nitrogen-containing fertilizer.	The process emission impact is 0.719 kg N / 1000 kg glucose. Process eutrophication emissions are mostly from phosphate fertilizer runoff during corn production. There is also a significant amount from ammonia emissions from nitrogen fertilizer in corn production.	n.a.	n.a.

Glycerol	n.a.	n.a.	n.a.	n.a.	n.a.
Sucrose	Prior to the biogenic emission credit, the impact from process emissions is 1808 kg CO_2eq / 1000. Of this, 94 %from CO_2. Most of this is from combustion of bagasse in the refining stage. This is mostly offset by a biogenic emissions credit during growth. Biogenic CO2 credit of -3192 kg/1000 kg. Due to sugarcane growth. Some of this is offset by bagasse combustion emissions.	A total of 5.29 kg SO_2eq / 1000 kg sucrose. This is from NO_x, SO_x, and ammonia emissions. About 70 % of the process emissions impact is from the CTG of sugarcane, and most of the rest is from the sucrose GTG.	The process emission impact is 5.58 kg N / 1000 kg sucrose. About 64 % of the process emissions impact is from sugar cane CTG, and 36 % is from sucrose GTG.	n.a.	The process emission impact is 111 kg O_3eq / 1000 kg sucrose. Most of this (> 99 %) is from Nox emissions to air. Of the process emission impact, 86 % is from sugar cane CTG, and 14 % is from the sucrose GTG. The sucrose GTG emissions are from combustion of bagasse for energy.
Sucralose	Prior to the biogenic emissions credit, the impact from process emissions is 4914 kg CO_2eq / 1000. Of this, 4468 kg is from CO_2. Much of this is from combustion of bagasse in the refining stage. This is mostly offset by a biogenic emissions credit during growth. 30% of the process GWP emissions are from the sucralose gtg, where CO2 is a	A total of 27.6 kg SO_2eq / 1000 kg sucralose. This is mostly from SO_x, NO_x, and ammonia. Small contributions are from HCl emissions to air. About 70 % of these process emissions are from phosgene CTG and sucrose CTGs. The sucrose emissions are mostly from the supply chain, but 28 % are from the gtg. The phosgene process	The process emission impact is 10.4 kg N / 1000 kg sucralose. Over 80 % of this is phosphate leaching. 92 % of the process emission impact is from the sucrose ctg. Of this, 36 % is from the gtg, and 64 % is from the CTG(sugarcane production).	n.a.	The process emission impact is 1513 kg O_3eq / 1000 kg sucralose. These are mostly from chlorine emissions to air, and most of these are in phosgene production. About 86 % of these emissions are in the phosgene gtg itself, and the other 14 % are in the supply chain.

	byproduct of the reaction chemistry. Biogenic CO_2 credit of -5531 kg/1000 kg. Due to sugarcane growth. Some of this is offset by bagasse combustion emissions.	emissions are all from the supply chain.			