Appendix 1

Table of allocation factors

Product	Economic allocation factors [%][1]	Mass allocation factors [%][2]
Titanium slag (chloride slag + sulfate slag)	81.01	69.42
Molten iron (HPPI + skimmed slag)	18.99	30.58
Chloride slag	85.70	77.53
Sulfate slag	14.30	22.47
High purity pig iron	99.86	95.69
Skimmed slag	0.14	4.31

Economic allocation factors are derived according to the following equations:

$$E.A.F_{Titanium\ slag} = \frac{\left(M.V_{Chlorine\ slag} \times P.V_{Chlorine\ slag}\right) + \left(M.V_{Sulfate\ slag} \times P.V_{Sulfate\ slag}\right)}{\sum(M.V \times P.V)_{All\ products}} \quad (1.2)$$

$$E.A.F_{Iron\ products} = \frac{(M.V_{HPPI} \times P.V_{HPPI}) + \left(M.V_{Skimmed\ slag} \times P.V_{Skimmed\ slag}\right)}{\sum(M.V \times P.V)_{All\ products}} \quad (1.3)$$

$$E.A.F_{Chlorine\ slag} = \frac{\left(M.V_{Chlorine\ slag} \times P.V_{Chlorine\ slag}\right)}{\sum(M.V \times P.V)_{titanium\ slag}} \quad (1.4)$$

$$E.A.F_{Sulfate\ slag} = \frac{\left(M.V_{Sulfate\ slag} \times P.V_{Sulfatelag}\right)}{\sum(M.V \times P.V)_{titanium\ slag}} \quad (1.5)$$

$$E.A.F_{HPPI} = \frac{(M.V_{HPPI} \times P.V_{HPPI})}{\sum(M.V \times P.V)_{Iron\ products}} \quad (1.6)$$

$$E.A.F_{Skimmed\ slag} = \frac{\left(M.V_{Skimmed\ slag} \times P.V_{Skimmed\ slag}\right)}{\sum(M.V \times P.V)_{Iron\ products}} \quad (1.7)$$

Where:

$$M.V = Market\ value$$
$$P.V = Production\ volume$$
$$Titanium\ slag = chlorine\ slag + sulfate\ slag$$

[1] Primary allocation factors
[2] Used in the sensitivity analysis

Appendix 2

LCI tables and H_2 production factors

Ilmenite mining and processing

Input from nature	*Unit*	*Amount*	*Background process*
Gangue	kg	1.61E+01	
Hafnium	kg	2.07E-03	
Iron	kg	9.85E-02	
Silicon	kg	3.19E-02	
Titanium	kg	1.35E-01	
Water, lake	m^3	1.46E-03	
Water, salt, ocean	m3	1.45E-04	
Water, unspecified natural origin	m3	6.13E-03	
Water, well	m3	6.63E-03	
Zirconium	kg	1.04E-01	
Occupation, mineral extraction site	m2a	1.03E-02	
Transformation from forest	m2	4.12E-04	
Transformation from pasture, man made	m2	6.18E-04	
Transformation, to mineral extraction site	m2	1.03E-03	
Inputs from technosphere			
Aluminum sulfate	kg	6.95E-05	Aluminium sulfate, without water, in 4.33% aluminium solution state {GLO}| market for | Cut-off, U
Lubrication oil	Kg	4.19E-04	Lubricating oil {RER}| market for lubricating oil | Cut-off, U
Mine infrastructure	p	1.53E-10	Mine infrastructure, bauxite {GLO}| market for | Cut-off, U
Recultivation	m^2	1.03E-03	Recultivation, bauxite mine {GLO}| market for | Cut-off, U
Sodium hydroxide	kg	3.71E-05	Sodium hydroxide, without water, in 50% solution state {GLO}| market for | Cut-off, U

Sulfuric acid	kg	9.91E-04	Sulfuric acid {RER}| market for sulfuric acid | Cut-off, U
Tap Water	kg	1.21E+00	Tap water {RoW}| market for | Cut-off, U & Tap water {ZA}| market for tap water | Cut-off, U
Water, harvested from rainwater	kg	7.50E-02	Water, harvested from rainwater {GLO}| market for water, harvested from rainwater | Cut-off, U
Diesel	MJ	2.52E-01	Diesel, burned in building machine {GLO}| market for | Cut-off, U
Electricity, medium voltage	kWh	8.97E-02	Electricity, medium voltage {SN}| market for electricity, medium voltage | Cut-off, U
Natural gas	MJ	1.28E-01	Heat, district or industrial, natural gas {RER}| market group for | Cut-off, U
Transportation	tkm	6	Transport, freight, sea, bulk carrier for dry goods {GLO}| transport, freight, sea, bulk carrier for dry goods | Cut-off, U

Outputs to technosphere

Ilmenite, 54% titanium dioxide	kg	1	Ilmenite, 54% titanium dioxide {RoW}| heavy mineral sand quarry operation | Cut-off, U

Emissions to air

CO2	kg	6.07E-02	
Particulates	kg	3.77E-05	
Radium-226	kBq	2.19E-05	
Thorium-232	kBq	1.37E-05	
Titanium	kg	7.57E-07	
Uranium-238	kBq	6.37E-06	
Water	m3	4.98E-03	
Zirconium	kg	7.63E-07	

Emissions to water

Suspended solids	kg	1.75E-05	
Titanium	kg	2.35E-08	
Water	m3	2.88E-03	

Waste treatment

Inert waste	kg	3.54E-02	Inert waste {Europe without Switzerland}| market for inert waste | Cut-off, U
Non-sulfidic overburden	kg	1.99E+00	Non-sulfidic overburden, off-site {GLO}| market for | Cut-off, U
Non-sulfidic tailing	kg	20.44E+00	Non-sulfidic tailing, off-site {GLO}| market for | Cut-off, U
Waste mineral oil	kg	3.72E-04	Waste mineral oil {Europe without Switzerland}| market for waste mineral oil | Cut-off, U
Wastewater	kg	1.28E-03	Wastewater, average {Europe without Switzerland}| market for wastewater, average | Cut-off, U

Production of green hydrogen from alkaline electrolysis (AEL)

Cell stack construction

Inputs from technosphere	*Unit*	*Amount*	*Background process*
Copper	t	2	Metal working, average for copper product manufacturing {GLO}| market for | Cut-off, U
Unalloyed steel	t	200	Steel, unalloyed {RER}| steel production, converter, unalloyed | Cut-off, U
Nickel	t	19	Nickel, class 1 {GLO}| processing of nickel-rich materials | Cut-off, U
Aluminium	kg	450	Aluminium alloy, AlMg3 {RER}| production | Cut-off, U
Calendered ridged plastic	kg	780	PVC calendered sheet E
Polytetrafluoroethylene	kg	78	Tetrafluoroethylene {RER}| production | Cut-off, U
Acrylonitrile butadiene styrene	kg	160	Acrylonitrile-butadiene-styrene copolymer {RER}| production | Cut-off, U
Polyphenylene sulfide	kg	340	Polyphenylene sulfide {GLO}| production | Cut-off, U
Polysulfones	kg	260	Polysulfone {GLO}| polysulfone production, for membrane filtration production | Cut-off, U
N-Methyl-2-pyrrolidone	t	1.3	N-methyl-2-pyrrolidone {RER}| production | Cut-off, U
Aniline	kg	49	Aniline {RER}| production | Cut-off, U
Acetic anhydride	kg	54	Acetic anhydride {RER}| production, ketene route | Cut-off, U
Terephthalic acid	kg	88	Purified terephthalic acid {RER}| production | Cut-off, U

Nitric acid	kg	33	Steam, in chemical industry {RER w/o RU}| nitric acid production, product in 50% solution state | Cut-off, U
Hydrochloric acid	kg	130	Hydrochloric acid, without water, in 30% solution state {RER}| market for | Cut-off, U
Graphite	kg	430	Graphite {RER}| production | Cut-off, U
Lubricating oil	kg	0.48	Graphite {RER}| production | Cut-off, U
Zirconium oxide	kg	1100	Zirconium oxide {RoW}| production | Cut-off, U
Carbon monoxide	kg	150	Carbon monoxide {RER}| production | Cut-off, U
Decarbonized water	t	11	Water, decarbonised {RoW}| water production, decarbonised | Cut-off, U
Deionized water	t	86	Water, deionised {Europe without Switzerland}| water production, deionised | Cut-off, U
Electricity	GJ	36	Electricity, medium voltage {Europe without Switzerland}| market group for | Cut-off, U
Heat	GJ	88	Heat, district or industrial, other than natural gas {Europe without Switzerland}| market for heat, district or industrial, other than natural gas | Cut-off, U
Steam	MJ	700	Steam, in chemical industry {RER}| market for steam, in chemical industry | Cut-off, U
Industrial machine production	kg	0.16	Industrial machine, heavy, unspecified {RER}| production | Cut-off, U
Plaster mixing	kg	780	Plaster mixing {RoW}| processing | Cut-off, U
Outputs to technosphere			
AEL 6MW	p	1	

Operation per MJ H_2 (AEL)

Inputs from technosphere	*Unit*	*Amount*	*Background process*
Electricity	MJ	1.5	Electricity, high voltage {NO}| Hydro, reservoir, alpine region | Cut-off, U
Deionized water	kg	8.34E-02	Water, deionised {Europe without Switzerland}| market for water, deionised | Cut-off, U
Nitrogen	g	2.42E-03	Nitrogen, liquid {RER}| air separation, cryogenic | Cut-off, U
Potassium hydroxide	g	1.58E-02	Potassium hydroxide {RER}| production | Cut-off, U
Steam	kg	9.18E-4	Steam, in chemical industry {RER}| production | Cut-off, U
Outputs to technosphere			
Hydrogen at 33 bars	MJ	1	
Emissions to air			
Oxygen	kg	6.62E-02	

H_2 conversion factors[1]

Gravimetric energy density (Lower heating value)	33.33 kWh/kg
Volumetric to gravimetric conversion factor	11.13 Nm3/kg
Energy conversion	3.6 MJ/ kWh

[1] National Academy of Sciences (2004). Access: https://nap.nationalacademies.org/read/10922/chapter/21

Alkaline production values (green H_2)[2]

Capacity per AEL	6 MW
System lifetime	20 years
Production rate	118 kg H2/h
Annual operation time	8300 h

$$Total\ production\ over\ the\ life\ time\ of\ 60\ MW\ AEL = Production\ rate * System\ lifetime * Annual\ operations * 10 * 3.6 = 23482094400\ MJ$$

[2] Koj et al. (2017)

LCI Blue and grey hydrogen production

Production of blue and grey H2 from SMR

Input from nature	*Unit*	*Blue Hydrogen*	*Grey hydrogen*	*Background process*
Water for cooling	m3	1.61E+01		
Inputs from technosphere				
Natural gas	m3	3.27E-02	3.27E-02	Natural gas, high pressure {NO}| petroleum and gas production, off-shore | Cut-off, U
Liquid storage tank	p	2.12E-11	2.10E-11	Liquid storage tank production, chemicals, organics RoW
Chemical factory	p	4.46E-12	4.46E-12	Chemical factory, organics {RER}| construction | Cut-off, U
Deionised water	kg	6.28E-02	6.28E-02	Water, deionised {Europe without Switzerland}| water production, deionised | Cut-off, U
Electricty, high voltage	kWh	4.12E-03	1.03E-04	Electricity, high voltage {NO}| market for | Cut-off, U
Diethanolamine	kg	1,61E-06		Diethanolamine {RER}| ethanolamine production | Cut-off, U
Aluminium oxide	kg	4.44E-06	4.44E-06	Aluminium oxide, metallurgical {IAI Area, EU27 & EFTA}| aluminium oxide production | Cut-off, U
Molybdenum	kg	1.39E-7	1.39E-07	Molybdenum {RER}| production | Cut-off, U
Zinc oxide	kg	3.09E-6	3.09E-6	Zinc oxide {RER}| production | Cut-off, U
Quicklime	kg	4.0E-07	4.0E-07	Quicklime, milled, packed {RER}| market for quicklime, milled, packed | Cut-off, U

Silica sand	kg	9.66E-8	9.66E-8	Silica sand {RoW}| production | Cut-off, U
Chromium oxide	kg	3.00E-07	3.0E-07	Chromium oxide, flakes {RER}| production | Cut-off, U
Copper oxide	kg	3.00E-06	3.00E-06	Copper oxide {RER}| production | Cut-off, U
Magnesium oxide	kg	2.33E-07	2.33E-07	Magnesium oxide {RER}| production | Cut-off, U
Portafer	kg	2.60E-06	2.60E-06	Portafer {RER}| production | Cut-off, U
Nickel	kg	1.69E-06	1.69E-06	Nickel, class 1 {GLO}| processing of nickel-rich materials | Cut-off, U
Zeolite	kg	7.36E-06	7.36E-06	Zeolite, powder {RER}| production | Cut-off, U
Transportation	tkm	2.29E-03	2.29E-03	Transport, freight, sea, tanker for liquefied natural gas {GLO}| transport, freight, sea, tanker for liquefied natural gas | Cut-off, U (Te 2023)

Outputs to technosphere			
Hydrogen, gaseous at 200 bar	MJ	1	1
Emissions to air			
Carbon dioxide, fossil	kg	2.60E-02	7.44E-02
Acetaldehyde	kq	2.35E-10	2.55E-10
Acetic acid	kq	3.52E-08	3.83E-08
Benzene	kg	9.39E-08	1.02E-07
Benzo(a)pyrene	kg	2.35E-12	2.55E-12
Butane	kq	1.64E-07	1.79E-07
Carbon monoxide, fossil	kg	4.93E-07	5.37E-07
Dinitrogen monoxide	kg	2.35E-08	2.56E-08

Formaldehyde	Kg	2.35E-08	2.56E-08
Mercury	Kg	7.04E-12	7.67E-12
Methane, fossil	Kg	4.70E-07	5.11E-08
Nitrogen dioxide, NO	Kg	4.20E-06	4.58E-06
PAH	Kg	2.35E-09	2.56E-09
Particulates, < 2.5 um	kg	4.70E-08	5.11E-08
Pentane	Kg	2.82E-07	3.07E-07
Propane	Kg	4.70E-08	5.11E-08
Propionic acid	Kg	4.70E-08	5.11E-09
Sulfur dioxide, NO	Kg	1.29E-07	1.41E-07
Toluene	Kg	4.70E-08	5.11E-08

Appendix 3

Tables of LCIA results for chloride slag, sulfate slag, HPPI and skimmed slag

Chloride slag – one kg

Impact catrgory	Unit	C-PR	H-PR Green H_2	H-PR Blue H_2	H-PR Grey H_2
Global warming	*kg CO_2eq*	1.52E+00	4.65E-01	5.38E-01	6.73E-01
Stratospheric ozone depletion	*kg CFC11eq*	2.99E-07	1.97E-07	1.97E-07	1.96E-07
Ozone formation. Human health	*kg NO_xeq*	3,29E-03	2.22E-03	2.24E-03	2.24E-03
Ozone formation. Terrestrial ecosystems	*kg NO_xeq*	3.98E-03	2.35E-03	2.40E-03	2.40E-03
Terrestrial acidification	*kg SO_2eq*	3.25E-03	2.26E-03	2.28E-03	2.28E-03
Terrestrial ecotoxicity	*kg 1,4-DCB*	1.80E+00	1.37E+00	1.44E+00	1.43E+00
Marine ecotoxicity	*kg 1,4-DCB*	2.82E-02	8.47E-03	1.00E-02	9.96E-03
Human non-carcinogenic toxicity	*kg 1,4-DCB*	8.11E-01	1.94E-01	2.07E-01	2.05E-01

Sulfate slag – 0.28 kg

Impact catrgory	Unit	C-PR	H-PR Green H_2	H-PR Blue H_2	H-PR Grey H_2
Global warming	*kg CO_2eq*	2.53E-01	7.75E-02	8.79E-02	1.12E-01
Stratospheric ozone depletion	*kg CFC11eq*	4.97E-08	3.11E-08	3.30E-08	3.27E-08
Ozone formation. Human health	*kg NO_xeq*	5.47E-04	3.66E-04	3.75E-04	3.74E-04
Ozone formation. Terrestrial ecosystems	*kg NO_xeq*	6.61E-04	3.79E-04	4.01E-04	4.01E-04
Terrestrial acidification	*kg SO_2eq*	5.41E-04	3.74E-04	3.81E-04	3.80E-04
Terrestrial ecotoxicity	*kg 1,4-DCB*	3.01E-01	2.28E-01	2.40E-01	2.39E-01
Marine ecotoxicity	*kg 1,4-DCB*	4.70E-03	1.41E-03	1.68E-03	1.66E-03
Human non-carcinogenic toxicity	*kg 1,4-DCB*	1.35E-01	3.24E-02	3.45E-02	3.41E-02

HPPI – 0.53 kg

Impact catrgory	Unit	C-PR	H-PR Green H_2	H-PR Blue H_2	H-PR Grey H_2
Global warming	*kg CO_2eq*	5.25E-01	1.97E-01	2.14E-01	2.54E-01
Stratospheric ozone depletion	*kg CFC11eq*	9.39E-08	5.93E-08	6.24E-08	6.19E-08
Ozone formation. Human health	*kg NO_xeq*	9.70E-04	6.48E-04	6.62E-04	6.61E-04
Ozone formation. Terrestrial ecosystems	*kg NO_xeq*	1.17E-03	6.77E-04	7.12E-04	7.12E-04
Terrestrial acidification	*kg SO_2eq*	9.73E-04	6.69E-04	6.82E-04	6.80E-04
Terrestrial ecotoxicity	*kg 1,4-DCB*	6.46E-01	4.66E-01	4.85E-01	4.84E-01
Marine ecotoxicity	*kg 1,4-DCB*	9.19E-03	3.31E-03	3.75E-03	3.72E-03
Human non-carcinogenic toxicity	*kg 1,4-DCB*	2.47E-01	7.04E-02	7.41E-02	7.32E-02

Skimmed slag – 0.024 kg

Impact catrgory	*Unit*	*C-PR*	*H-PR Green H_2*	*H-PR Blue H_2*	*H-PR Grey H_2*
Global warming	kg CO_2 eq	7.18E-04	2.78E-04	3.06E-04	3.57E-04
Stratospheric ozone depletion	kg CFC11 eq	1.28E-10	8.74E-11	8.78E-11	8.72E-11
Ozone formation. Human health	kg NOx eq	1.33E-06	9.22E-07	9.33E-07	9.32E-07
Fine particulate matter formation	kg PM2.5 eq	1.60E-06	9.82E-07	1.00E-06	1.00E-06
Ozone formation. Terrestrial ecosystems	kg NOx eq	1.33E-06	9.49E-07	9.61E-07	9.57E-07
Terrestrial acidification	kg SO2 eq	8.83E-04	6.57E-04	6.83E-04	6.82E-04
Terrestrial ecotoxicity	kg 1.4-DCB	1.26E-05	4.67E-06	5.29E-06	5.24E-06
Marine ecotoxicity	kg 1.4-DCB	3.38E-04	9.91E-05	1.04E-04	1.03E-04
Human non-carcinogenic toxicity	kg 1.4-DCB	7.18E-04	2.78E-04	3.06E-04	3.57E-04
Mineral resource scarcity	kg Cu eq	1.28E-10	8.74E-11	8.78E-11	8.72E-11

Appendix 4

Contribution analysis results

Contribution analysis - Ilmenite MPT

Per kg chloride slag

	Total	Ilmenite mining and processing	Recultivation of mine	Transport	Diesel	Electricity	Heat, natural gas	Mine infrastructure	Inert waste	Wastewater	Other
GWP	2.52E-01	2.67E-02	1.74E-02	4.57E-02	3.24E-02	1.14E-01	9.29E-03				6.47E-03
Stratospheric ozone depletion	1.52E-07		1.02E-08	2.95E-08	1.90E-08	8.50E-08					7.95E-09
Ozone formation, human health	1.94E-03		2.13E-04	9.20E-04	3.95E-04	3.86E-04					2.69E-05
Ozone formation, terrestrial ecotoxicity	1.96E-03		2.15E-04	9.28E-04	4.02E-04	3.89E-04					2.99E-05
Terrestrial acidification	2.06E-03		9.61E-05	9.75E-04	1.80E-04	7.58E-04					4.87E-05
Terrestrial ecotoxicity	6.64E-01		2.03E-02	1.48E-01	3.80E-02	4.19E-01					3.95E-02
Marine ecotoxicity	3.71E-03		1.19E-04	7.88E-04	2.22E-04	1.49E-03		2.05E-04	5.18E-04		3.74E-04
Human non-carcinogenic toxicity	6.31E-02		1.60E-03	8.32E-03	2.99E-03	1.87E-02		2.94E-03	1.88E-02	4.90E-03	4.87E-03

Contribution analysis – Pre-reduction C-PR

Per kg chloride slag

	Total	Direct emissions[a7]	Grinding balls	Bentonite	Grinding balls	Diesel	Zinc dust	Heat	Other
GWP	1.00E+00	9.97E-01							6.11E-03
Stratospheric ozone depletion	2.83E-09		5.57E-10	2.03E-09	4.43E-10	8.03E-11	-0.0876515	-3.63E-11	-2.89E-17
Ozone formation, human health	2.03E-04	1.79E-04	3.43E-06	1.55E-05	5.89E-06				-1.64E-06
Ozone formation, terrestrial ecotoxicity	5.88E-04	5.64E-04		1.58E-05					8.24E-06
Terrestrial acidification	2.47E-04	2.27E-04		1.40E-05					6.94E-06
Terrestrial ecotoxicity	6.66E-01	6.66E-01		4.10E-02			-2.088E-05		1.52E-02
Marine ecotoxicity	2.70E-04	1.76E-03	8.62E-05	1.10E-04	1.78E-04		-4.5806671	-5.39E-04	5.31E-04
Human non-carcinogenic toxicity	5.46E-02	9.94E-02	0.00E+00	1.64E-03	2.19E-03		-0.0002452		1.09E-03

Contribution analysis – Smelting in EAF C-PR

Per kg chloride slag

	Total	Direct emissions[a]	Hard coal	Anthracite	Electrode paste	Taphole clay	Electricity Hydropower	Other
GWP	1.65E-01	1.27E-01	1.21E-02	1.16E-02	2.97E-03		9.06E-03	1.93E-03
Stratospheric ozone depletion	7.00E-08	5.20E-08	5.06E-09	4.86E-09	2.86E-09		4.15E-09	1.11E-09
Ozone formation, human health	2.57E-04	1.21E-04	4.89E-05	4.69E-05	9.93E-06		2.55E-05	4.50E-06
Ozone formation, terrestrial ecotoxiity	5.19E-04	3.80E-04	4.97E-05	4.77E-05	1.10E-05		2.61E-05	4.57E-06
Terrestrial acidification	2.07E-04	8.59E-05	3.69E-05	3.54E-05	1.79E-05	6.49E-06	2.27E-05	1.36E-06
Terrestrial ecotoxicity	3.25E-01	2.28E-01	1.13E-02	1.09E-02	1.74E-02		4.94E-02	8.01E-03
Marine ecotoxicity	4.72E-03	1.79E-04	1.88E-03	1.81E-03			6.45E-04	2.06E-04
Human non-carginogenic toxicity	1.38E-01	1.98E-02	5.38E-02	5.16E-02			9.83E-03	3.26E-03

Contribution analysis – Slag refining C-PR

Per kg chloride slag

	Total	Direct emissions[a]	Diesel production	Electricity Hydropower
GWP	5.32E-03	5.32E-03	5.32E-03	5.32E-03
Stratospheric ozone depletion	1.37E-09	1.37E-09	1.37E-09	1.37E-09
Ozone formation, human health	8.13E-06	8.13E-06	8.13E-06	8.13E-06
Ozone formation, terrestrial ecotoxicity	1.88E-05	1.88E-05	1.88E-05	1.88E-05
Terrestrial acidification	3.39E-05	3.39E-05	3.39E-05	3.39E-05
Terrestrial ecotoxicity	8.57E-03	8.57E-03	8.57E-03	8.57E-03
Marine ecotoxicity	3.60E-05	3.60E-05	3.60E-05	3.60E-05
Human non-carcinogenic toxicity	6.66E-04	6.66E-04	6.66E-04	6.66E-04

Contribution analysis – Pre-reduction H-PR

Per kg chloride slag

	Total	Direct emissions[a]	Natural gas	Electricity	Nitrogen	Other
GWP	1.57E-01	1.47E-01	8.60E-03			1.70E-03
Stratospheric ozone depletion	8.97E-09	3.60E-09	3.60E-09	3.28E-10	1.45E-09	3.49E-13
Ozone formation, human health	1.17E-04	7.63E-05	3.57E-05			4.72E-06
Ozone formation, terrestrial ecotoxicity	1.99E-05	1.29E-05	6.20E-06			8.08E-07
Terrestrial acidification	5.22E-05	2.89E-05	1.90E-05		2.51E-06	1.79E-06
Terrestrial ecotoxicity	4.49E-01	3.84E-01	4.67E-02		1.41E-02	3.90E-03
Marine ecotoxicity	1.87E-03	1.02E-03	6.81E-04	5.10E-05	1.19E-04	5.12E-11
Human non-carcinogenic toxicity	6.23E-02	5.75E-02	2.94E-03			1.83E-03

Contribution analysis – Smelting in EAF H-PR

Per kg chloride slag

	Total	Direct emissions[a]	Hard coal	Anthracite	Electrode paste	Taphole clay	Electricity Hydropower	Other
GWP	4.30E-02	2.47E-02	3.15E-03	4.78E-03	2.50E-03	1.11E-03	6.43E-03	2.80E-04
Stratospheric ozone depletion	8.97E-09	4.67E-09	6.03E-10	9.16E-10	1.10E-09		1.35E-09	3.33E-10
Ozone formation, human health	1.17E-04	3.24E-05	1.74E-05	2.64E-05	1.14E-05	3.34E-06	2.47E-05	1.05E-06
Ozone formation, terrestrial ecotoxicity	1.99E-05	1.07E-05	1.86E-06	2.82E-06	1.32E-06		2.66E-06	4.69E-07
Terrestrial acidification	5.22E-05	1.13E-05	6.43E-06	9.76E-06	1.01E-05		9.36E-06	5.25E-06
Terrestrial ecotoxicity	4.49E-01	3.06E-01			3.37E-02		8.05E-02	2.83E-02
Marine ecotoxicity	1.87E-03	1.00E-04	4.70E-04	7.14E-04	6.85E-05		4.39E-04	7.87E-05
Human non-carcinogenic toxicity	5.59E-02	1.15E-02	1.39E-02	2.11E-02	7.81E-04		6.92E-03	1.67E-03

Contribution analysis – Slag refining H-PR

Per kg chloride slag

	Total	Direct emissions[a]	Electricity Hydropower
GWP	1.31E-04		1.31E-04
Stratospheric ozone depletion	5.99E-11		5.99E-11
Ozone formation, human health	3.68E-07		3.68E-07
Ozone formation, terrestrial ecotoxiity	3.77E-07		3.77E-07
Terrestrial acidification	3.27E-07		3.27E-07
Terrestrial ecotoxicity	3.51E-03	2.80E-03	7.13E-04
Marine ecotoxicity	1.61E-05	6.75E-06	9.31E-06
Human non-carginogenic toxicity	2.85E-04	1.43E-04	1.42E-04

Contribution analysis – Coal MPT

Per kg chloride slag

	Total	Coal mining and processing	Transport	Other
GWP	9.75E-02	8.22E-02	1.53E-02	6.45E-10
Stratospheric ozone depletion	7.32E-08	6.12E-08	1.20E-08	2.32E-16
Ozone formation, human health	8.78E-04	5.09E-04	3.69E-04	1.80E-11
Ozone formation, terrestrial ecotoxiity	8.91E-04	5.17E-04	3.74E-04	1.43E-11
Terrestrial acidification	7.29E-04	4.58E-04	2.71E-04	7.90E-12
Terrestrial ecotoxicity	1.42E-01	7.14E-02	7.01E-02	
Marine ecotoxicity	1.94E-02	1.88E-02	6.46E-04	3.72E-11
Human non-carginogenic toxicity	5.55E-01	5.45E-01	9.32E-03	6.75E-09

Contribution analysis – Green H2 production

Per kg chloride slag

	Total	AEL	Electricity	Steam	Water deionized	Other
GWP	9.20E-03	5.82E-04	7.68E-03	7.42E-04		2.00E-04
Stratospheric ozone depletion	4.46E-09	6.14E-10	3.52E-09	1.84E-10		1.44E-10
Ozone formation, human health	2.47E-05	1.70E-06	2.16E-05	8.97E-07		4.56E-07
Ozone formation, terrestrial ecotoxiity	2.53E-05	1.79E-06	2.21E-05	9.20E-07		4.65E-07
Terrestrial acidification	2.38E-05	1.88E-06	1.92E-05	1.68E-06	7.04E-07	3.57E-07
Terrestrial ecotoxicity	4.80E-02	3.67E-03	4.19E-02			2.41E-03
Marine ecotoxicity	8.91E-04	3.21E-04	5.47E-04			2.33E-05
Human non-carginogenic toxicity	1.17E-02	3.01E-03	8.33E-03			4.01E-04

Contribution analysis – Blue H2 production

Per kg chloride slag

	Total	SMR w. CCS	Natural gas	Chemical factory	Electricity	Copper oxide	Transport	Other
GWP	8.16E-02	7.30E-02	6.25E-03					2.38E-03
Stratospheric ozone depletion	4.47E-09	7.25E-10	1.83E-09	7.95E-10	7.95E-10			3.28E-10
Ozone formation, human health	4.92E-05	1.24E-05	2.81E-05	5.38E-06			1.60E-06	1.79E-06
Ozone formation, terrestrial ecotoxiity	7.68E-05	3.86E-05	2.93E-05	5.51E-06				3.46E-06
Terrestrial acidification	4.40E-05	9.43E-06	1.32E-05	1.51E-05		2.84E-06	1.59E-06	1.93E-06
Terrestrial ecotoxicity	1.16E-01		4.36E-03	8.55E-02		2.30E-02		3.50E-03
Marine ecotoxicity	2.38E-03		5.97E-04	1.31E-03		3.22E-04		1.55E-04
Human non-carginogenic toxicity	2.24E-02		1.32E-03	1.57E-02		3.73E-03		1.62E-03

Contribution analysis – Grey H2 production

Per kg chloride slag

	Total	SMR w. CCS	Natural gas	Chemical factory	Copper oxide	Transport	Other
GWP	2.17E-01	2.09E-01	6.35E-03				2.15E-03
Stratospheric ozone depletion	3.79E-09	7.89E-10	1.86E-09	7.95E-10			3.45E-10
Ozone formation, human health	5.03E-05	1.35E-05	2.85E-05	5.38E-06		1.60E-06	1.36E-06
Ozone formation, terrestrial ecotoxiity	8.03E-05	4.20E-05	2.97E-05	5.51E-06			3.02E-06
Terrestrial acidification	4.46E-05	1.03E-05	1.34E-05	1.51E-05	2.83E-06	1.59E-06	1.45E-06
Terrestrial ecotoxicity	1.16E-01		4.43E-03	8.55E-02	2.29E-02		2.81E-03
Marine ecotoxicity	2.37E-03		6.06E-04	1.31E-03	3.19E-04		1.41E-04
Human non-carginogenic toxicity	2.22E-02		1.34E-03	1.57E-02	3.71E-03		1.40E-03

Direct emissions from gate-to-gate processes[a]

	Unit process		Unit	CO2	N2O	CH4	Nox	NMVOC	SO2	Copper to air	Copper to water	Lead to air	Lead to water	Vanadium to air	Zinc to air	Zinc to water	Arsenic to air	Arsenic to water	Nickel to air	Nickel to water	Mercury to air	Chromium to air	Other
GWP	Pre-reduction	C-PR	%	100																			
		H-PR	%	99		1																	
	Smelting	C-PR	%	99	1																		
		H-PR	%	99	1																		
	Slag refining	C-PR	%	98		1																	
Stratospheric ozone depletion	Pre-reduction	C-PR	%																				
		H-PR	%																				
	Smelting	C-PR	%		100																		
		H-PR	%		100																		
	Slag refining	C-PR	%																				
Ozone formation, human health	Pre-reduction	C-PR	%		99																		1
		H-PR	%				95	3															2
	Smelting	C-PR	%				100																
		H-PR	%				10																
	Slag refining	C-PR	%		97	3																	
Ozone formation, terrestrial ecotoxicity	Pre-reduction	C-PR	%		99																		1
		H-PR	%				97	2															
	Smelting	C-PR	%				100																
		H-PR	%				100																
	Slag refining	C-PR	%		98			2															
	Pre-reduction	C-PR	%				56		44														
		H-PR	%						100	10		8		3	79								

Terrestrial acidification	Smelting	C-PR	%				100															
		H-PR	%																			
	Slag refining	C-PR	%				93		7													
Terrestrial ecotoxicity	Pre-reduction	C-PR	%							10		8		3	78						1		1
		H-PR	%							10		8		3	79								1
	Smelting	C-PR	%							10		8		3	77				1				
		H-PR	%							10		8		3	77				1				1
	Slag refining	C-PR	%							1				86	1				0			12	
		H-PR	%							1				86	1							12	
Marine ecotoxicity	Pre-reduction	C-PR	%							2	1				25	68				2			
		H-PR	%							2	1			1 %		68				2			
	Smelting	C-PR	%												84	3				3			11
		H-PR	%							6					84	3							5
	Slag refining	C-PR	%								1			30		67							2
		H-PR	%								1			29		67			1				
Human non-carcinogenic toxicity	Pre-reduction	C-PR	%									27			32	33	1	6					1
		H-PR	%									27			32	33	1	6					1
	Smelting	C-PR	%									45			54	1							1
		H-PR	%									45			54	1							1
	Slag refining	C-PR	%									0	2	6	1	87		4					
		H-PR	%										2	6	1	87		4					

Appendix 5

Calculations of emissions from burning of natural gas by employing emission factors from SSB

NG consumption	21 756 000	kg
	29 400 000	sm3
Assumed source	**S.01 Direct fired furnaces**	

NO_X Natural gas

Emission factor	5.95	kg NOx / 1000 sm3 NG
Emission faktor	0.00595	kg NOx/Sm3
Density NG	0.740	kg NG/Sm3
Emission factor	0.008040541	kg Nox/ kg NG
Calculated emission	174930	kg
Estimated emission	5141.411081	

C-PR Pre-reduction	40240.78313	kg NOx
Emission factor coal furnace	16	kg NOx/ton coal
Total emissions	1369141.678	kg
Capture rate	97 %	
Emission rate	0.029391248	

CH4 Natural gas

Emission factor	0.1775	kg CH4/ 1000 sm3 NG
Emission factor	0.0001775	kg CH4/ sm3 NG
Emission factor	0.000239865	kg CH4 / kg NG
Calculated emission	5218.5	kg

N2O Natural gas

Emission factor	0.0036	kg/ 1000 sm3 NG
Emission factor	0.0000036	kg/ sm3 NG

Calculated emission	105.84	kg

CO2 - Stationary and mobile combustion		
Emission factor	1.99	ton CO2/ 1000 sm3 NG
	1.99	kg CO2/ sm3
	2.689189189	kg CO2 / kg NG
	58 506 000	kg CO2

PM Natural gas		
Emission factor	0.122	kg/ 1000 sm3 NG
Emission factor	0.000122	kg/ sm3 NG
Calculated emission	2.1655E-08	kg

Heavy metals			**Conversion**		**Total**	
Pb	0.00025	g/1000 sm3	2.5E-10	kg/ sm3	5.44E-03	kg
Cd	0.002	g/1000 sm4	0.000000002	kg/ sm3	4.35E-02	kg
Hg	0.001	g/1000 sm5	0.000000001	kg/ sm3	2.18E-02	kg
As	0.004	g/1000 sm6	0.000000004	kg/ sm3	8.70E-02	kg
Cr	0.021	g/1000 sm7	0.000000021	kg/ sm3	4.57E-01	kg
Cu	0.016	g/1000 sm8	0.000000016	kg/ sm3	3.48E-01	kg

PAH						
Benzo(a)pyrene	0.00002	g/1000 sm3	2E-11	kg/ sm3	4.35E-04	kg
Benzo(b)fluoranthene	0.00003	g/1000 sm4	3E-11	kg/ sm3	6.53E-04	kg
benzo(k)fluoranthene	0.00003	g/1000 sm5	3E-11	kg/ sm3	6.53E-04	kg
indeno(1 ,2,3_cd) pyrene	0.00003	g/1000 sm6	3E-11	kg/ sm3	6.53E-04	kg

Appendix 6

Emission factors per kg H_2

GWP used in H_2 sensitivity analysis

[kg CO_2eq per kg H_2]	**Green H_2**	**Blue H_2**	**Grey H_2**
Hydropower (base-case)	0.39		
Hydropower Norsus	0.23		
NO market mix	1.03		
NORDEL	2.97		
ENTSO-E	18.90		
CCS 90% (base-case)		3.49	
CCS 98%		2.98	
Original background processes		4.93	10.6
Low CH_4 (0.2%)		2.70	10.3
High CH_4 (8%)		9.00	17.0
NO grey (base-case)			9.28

Appendix 7

Evaluation of completeness, consistency, and representativeness of the foreground system

Data quality	Criteria	Comment	Significant issues
Completeness	All environmentally relevant material and energy flows within the system boundary must be included.	No cut-off criteria were used during data collection.	Dataset for the production of "smetemasse" was not found, and as a result, it was not included in the background system. Storage of H2 is not included as part of the system boundary.
Consistency	Assumptions, methods, and data should be applied consistently to the various components in the analysis.	Methodological choices have been discussed and assessed in Chapter 7. Allocation methods have been applied consistently for all gate-to-gate unit processes.	The allocation method applied for ilmenite is based on physical factors and not economic. Regarding green H2 production, no pressurization is not included.
Geographical representativeness	The data used should accurately reflect the geographical region of the process in line with the G&S.	Data collected for the gate-to-gate unit processes are regarded as very good in terms of geographical representativeness as primary data was collected. Ilmenite mining and processing and H2 production processes are regarded as good in terms of geographical representativeness. The processes are based on secondary data and efforts have been made to increase the geographical representativeness by replacing generic background processes. Each dataset used as background data is evaluated separately in the following table.	Dataset used for mining and processing of ilmenite is averaged for several facilities.
Technological representativeness	The data used should accurately reflect the specific technology used in the investigated process.	Data collected for ilmenite, gate-to-gate processes and green H2 production are regarded as very good in terms of technological representativeness. Each dataset used as background data is evaluated separately in in the following table.	Significant uncertainties exist regarding the technological aspects of CCS for blue H2 production. Some of these have been assessed in the sensitivity analysis.

Temporal representativeness	The data used should be representative in terms of age and collected over an adequate period of time.	Data collected for the foreground system is regarded as very good in terms of temporal representativeness. Each dataset used as background data is evaluated separately in in the following table.	Annual data for all gate-to-gate unit processes have only been collected for a one-year period.

Criteria for evaluation of the representativeness of background processes

Points	Criteria	Context
Geographical		
1	IF a specific producer is provided: process modeled for RoW, OR the wrong specific country	A
	IF a specific producer is not provided: the process is modeled for RoW	B
2	IF a specific producer is provided: Process modeled for the same region OR the specific producer is a part of an averaged process	A
	IF a specific producer is not provided: Process modeled for the most probable market	B
3	IF a specific producer is provided: Process modeled for the same country as the place of production	A
	IF a specific marked is provided: Process modeled for the correct marked	B
	IF a specific producer is provided: Process modeled for the specific producer	C
	IF a specific producer is provided: Process has been adapted to represent the specific country as the place of production	D
Technical/ temporal		
1	IF specific producer and technology is identified: Process is modeled using very different technology/ equipment (i.e. proxy) OR high uncertainty of available process	A
	IF specific producer and technology is not identified: Process is modeled using outdated technology that is not representative of the current production method OR high uncertainty of available process	B

2	IF specific producer and technology/ production method is identified: Modeled using similar process technology/ method/ equipment as the specific producer OR modeled as an average of different technologies/ processes inc., the specific producer	A
	IF specific producer and technology is not identified: Modeled using "common" or average process technology	B
3	IF specific producer and technology/ production method is identified: modeled using the same process technology/ method/ equipment as the specific producer	A
	IF specific producer and technology is not identified: Modeled using mature production methods/ technology that can be assumed to be the general technology/ production method	B

Evaluation of the representativeness of background processes

Background process	Assessment indicator		Alterations
	Geographical representativeness	Technological/ temporal representativeness	
Hard coal {Europe, without Russia and Turkey}| hard coal, import from RU | Cut-off, U	3B	3B	
Hard coal {Europe, without Russia and Turkey}| hard coal, import from RLA | Cut-off, U	3A	3A	
Diesel {Europe without Switzerland}| diesel production, petroleum refinery operation | Cut-off, U	3B	2B	
Bentonite {RoW}| quarry operation | Cut-off, U (Te 2023)	1A	2B	
Taphole cley for ferrotitanium plant	3C	3A	
Cast iron {RER}| production	2B	3B	
Electricity, high voltage {NO}| Hydro, reservoir, alpine region | NO hydropower | Cut-off, U	3B	3A	
Bulk lead-zinc concentrate {GLO}| zinc mine operation | Cut-off, U	2B	Substitute	
Nitrogen, liquid {RER}| air separation, cryogenic | Cut-off, U	2A	2B	
Aluminium sulfate, powder {RER}| production | Cut-off, U	2B	2B	
Anode, paste, for aluminium electrolysis {IAI Area, EU27 & EFTA}| anode production, paste, for aluminium electrolysis | Cut-off, U	2A	2A	
Petroleum coke {Europe without Switzerland}| petroleum coke production, petroleum refinery operation | Cut-off, U	3D	2B	Petroleum and natural gas processes have been substituted with processes specific to production country
Propane {RoW}| natural gas production | Cut-off, U	1B	3B	
Calcium carbide, technical grade {RER}| production | Cut-off, U	3D	1B	Electricity substituted with market mix specific to production country

			Quicklime substituted with market process specific to production region
Magnetite {GLO}| ilmenite - mine operation | Cut-off, U	3D	2B	Electricity substituted with market mix specific to production country
Calcium carbonate, precipitated {RER}| calcium carbonate production, precipitated | Cut-off, U	2A	2B	
Ferrosilicon {RoW}| production | Cut-off, U	3D	2A	Electricity and natural gas substituted for processes specific to production country Heavy fuel oil and hard coal substituted with processes specific to production region