

Supplementary Information for

Evaluating the possibilities and limitations of the pyrometallurgical recycling of waste Li-ion batteries using simulation and life cycle assessment

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S1. Modeling

The flowsheets drawn in HSC Sim, the most important assumptions in the model, as well as the process parameters are listed in the subsections.

S1.1. Flowsheets

The flowsheets (**Figure S1-S3**) are the same for all the scenarios. In the LFP scenarios, the solvent extraction circuits for impurities, cobalt, and nickel are turned off so that no pure solution forms (i.e., the aqueous phase passes the extraction units in the model without changes).

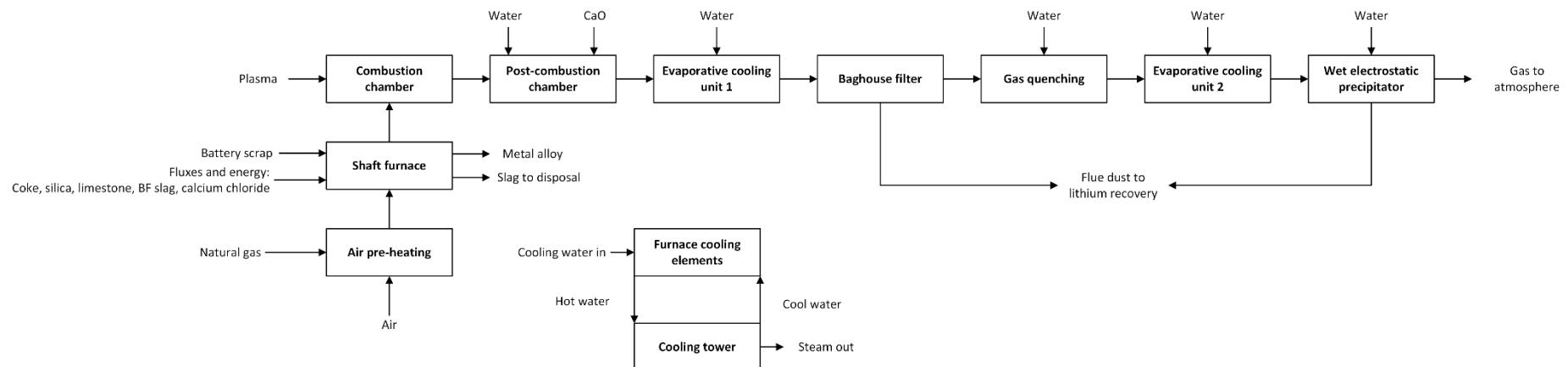


Figure S1. Blocksheet for the pyrometallurgical process with all the inputs and outputs.

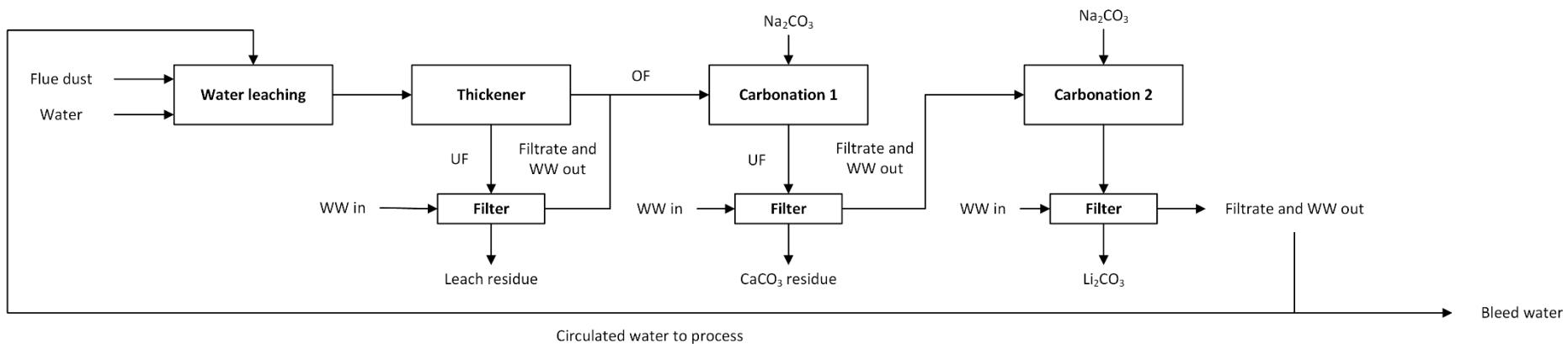


Figure S2. Blocksheet for lithium recovery with all the inputs and outputs. UF = underflow, OF = overflow, WW = washwater.

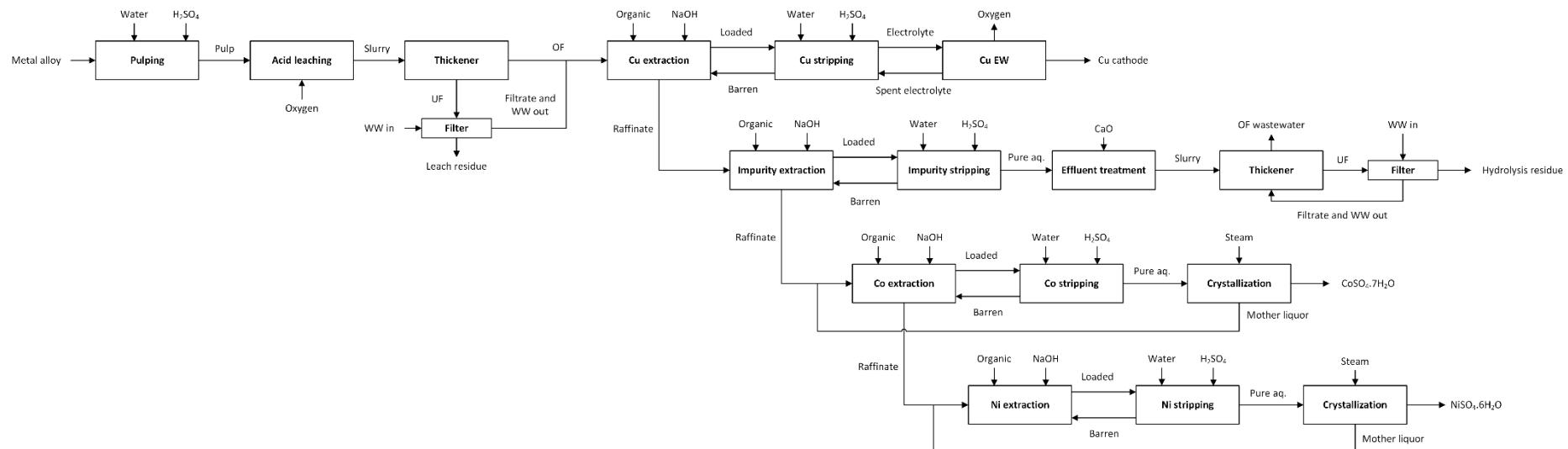


Figure S3. Blocksheet for alloy refining with inputs and outputs. "Loaded" refers to metal-loaded organic, "Barren" to stripped organic, and "Pure/Impurity aq." to purified strip solution.

S1.2. Assumptions

The entirety of the process flowsheet is not operated anywhere as it was modeled, but it consists of a combination of industrially implemented and novel unit processes. The technologies themselves are established: although lithium has, to the authors' knowledge, not so far been recovered commercially by volatilization, the separation of metals based on their volatility is industrially utilized, for instance, in the processing of zinc and lead-bearing raw materials (Hoang et al., 2009).

The slag chemistry and the mass balance were modeled based on the examples by Cheret and Santén (2005), which showed high variability: for example, the slag/alloy mass ratio varied between 1.3-6.7 kg/kg. It is also stated that the SiO₂/CaO ratio should be preferably at least 1.5, and that alumina content should be below 25 wt.% to avoid problems caused by high slag viscosity. The slag was modeled differently between LFP and NMC feeds. For NMC, three controls were used: slag/alloy ratio, SiO₂ content in the slag, and SiO₂/CaO ratio. For LFP, the slag was needed to dissolve phosphorus and iron in addition to aluminum, so only the SiO₂ content and SiO₂/CaO ratio were controlled.

The mass balance of lithium-ion battery smelting has been reported between the metal alloy and slag, but the composition of the flue dust is less clear. Qu et al. (2022) studied the smelting volatilization of lithium from pre-treated battery scrap with industrial copper slag and characterized the flue dust with XRD. The characterization showed lithium chloride, sodium chloride, zinc oxide, and lead, making it reasonable to expect that mainly halides would be present in the simulated dust given that zinc and lead in the study by Qu et al. (2022) originated from the copper slag. Calcium oxide was selected over sodium hydroxide for binding fluoride and chloride since calcium fluoride is practically insoluble in water, and CaO has been shown an effective sorbent for hydrogen fluoride (Byer et al., 1983).

The gas cleaning system after fluoride removal was assumed to consist of a series of evaporative cooling units, baghouse filter, and wet electrostatic precipitator (W-ESP). A heat recovery boiler was not considered, so steam for the process was assumed to be generated in other ways. The temperature of the gas was presumed to decrease incrementally to 40 °C in the cooling systems, and altogether 99% of solid particles was captured.

The solvent extraction circuits were modeled with only one extraction and stripping unit each, without including scrubbing stages. The actual number of extraction and stripping stages would need to be confirmed experimentally. The heat balance of the SX units was not modeled since the organics added to the database did not have heat capacity constants, leading to erroneous enthalpy balances.

The model had to be modified for different feeds to keep the LCI consistent. The most obvious example is that the alloy from LFP scenarios does not contain cobalt or nickel, so the solvent extraction circuits after copper recovery were turned off.

S1.3. Model parameters

The main parameters used in the models are provided in **Table S1** for the pyrometallurgical and gas cleaning units, including lithium recovery from flue dust.

Table S1. Process parameters for the pyrometallurgical process, gas cleaning, and lithium recovery.

Unit	Parameter	Value	Ref.
Air pre-heating	Temperature	500 °C with natural gas	Cheret and Santén (2005)
Reduction smelting	Temperature	1450 °C slag; 1450 °C alloy; 700 °C gas	Cheret and Santén (2005)
Reduction smelting	SiO ₂ /CaO ratio in slag	1-1.5 to >1.5 wt/wt (used 1.5)	Cheret and Santén (2005)
Reduction smelting	SiO ₂ in slag	~50 wt.%	Estimate
Reduction smelting	Slag/alloy ratio (NMC)	~4 kg/kg	Estimate
Reduction smelting	Al ₂ O ₃ in slag	<25 wt.%	Cheret and Santén (2005)
Reduction smelting	Mn distribution between slag and alloy	2 wt.% in alloy	Cheret and Santén (2005)
Reduction smelting	Fe distribution between slag and alloy	4 wt.% in alloy	Cheret and Santén (2005)
Reduction smelting	Li/CaCl ₂ ratio	20% chloride excess	Scheunis and Callebaut (2019)
Reduction smelting	Heat losses	10% input enthalpy	Estimate
Combustion chamber	Gas temperature	1150 °C (by heating)	Cheret and Santén (2005)
Post-combustion	Gas temperature	300 °C (water-cooled)	Cheret and Santén (2005)
Post-combustion	CaO feed	Stoichiometric (100% HF and HCl converted)	Estimate
Gas cleaning line	Dust removal efficiency	99%	Estimate
Gas cleaning line	Gas exit temperature	40 °C	Estimate
Lithium leaching	S/L ratio	50 g/L	Estimate
Lithium leaching	Temperature	80 °C	Estimate
Lithium leaching	CaF ₂ solubility	0.016 g/L in water	HSC database
First carbonation	Na ₂ CO ₃ feed	1 mol Na ₂ CO ₃ : 1 mol Ca	Estimate
First carbonation	CaCO ₃ extraction	CaCO ₃ solubility ~20 mg/L	HSC database
Second carbonation	Na ₂ CO ₃ feed	0.5 mol Na ₂ CO ₃ : 1 mol Li	Estimate
Second carbonation	Temperature	80 °C	An et al. (2012)
Second carbonation	Li ₂ CO ₃ extraction	Li solubility 1.8 g/L	An et al. (2012)

The main parameters for the hydrometallurgical refining of pyrometallurgically produced copper-nickel-cobalt alloy are presented in **Table S2**. Solid/liquid separation units: thickeners and filters, were modeled with the default constants in HSC Sim. Cobalt and nickel crystallization were simulated using their solubility in sulfuric acid solutions (Charykova et al., 2010; Kobylin et al., 2013).

The LFP scenarios were modeled without controls in the circuits after copper extraction, and all of the raffinate from copper SX was subjected to neutralization prior to discharge.

Table S2. Process parameters for alloy refining.

Unit	Parameter	Value	Ref.
Leaching	H ₂ SO ₄ concentration	2 mol/L	Calculated consumption
Leaching	S/L ratio	100 g/L	Xiao et al. (2017)
Leaching	Temperature	90 °C	Xiao et al. (2017)
Leaching	Oxygen utilization efficiency	30%	Estimate
Cu SX - extraction	pH	2	Sahu et al. (2004)
Cu SX - extraction	O/A ratio	1:1 vol/vol	Estimate
Cu SX - extraction	LIX 84-I concentration	0.1 M in kerosene	Sahu et al. (2004)
Cu SX - stripping	O/A ratio	Cu concentration in aqueous (~45-50 g/L)	Schlesinger et al. (2022)
Cu SX - stripping	H ₂ SO ₄ concentration	175 mol/l	Schlesinger et al. (2022)
Cu electrowinning	[Cu ²⁺] in advance electrolyte	~45 g/L calculated in the model	Schlesinger et al. (2022)
Cu electrowinning	[Cu ²⁺] in spent electrolyte	Advance electrolyte -5 g/L (~40 g/L)	Schlesinger et al. (2022)
Impurity SX - extraction	pH	3.0	Tang et al. (2023)
Impurity SX - extraction	O/A ratio	1:1 vol/vol	Tang et al. (2023)
Impurity SX - extraction	D2EHPA concentration	1 mol/L in kerosene	Tang et al. (2023)
Impurity SX - stripping	O/A ratio	1.5:1	Tang et al. (2023)
Impurity SX - stripping	H ₂ SO ₄ concentration	0.5 M in feed	Tang et al. (2023)
Co SX - extraction	pH	5.5	Tang et al. (2023)
Co SX - extraction	O/A ratio	1:1 vol/vol	Tang et al. (2023)
Co SX - extraction	Cyanex 272 in kerosene	0.4 M	Tang et al. (2023)
Co SX - extraction	TBP in kerosene	5 vol.%	Tang et al. (2023)
Co SX - stripping	O/A ratio	1:1	Tang et al. (2023)
Co SX - stripping	H ₂ SO ₄ concentration	0.1 mol/L	Tang et al. (2023)
Ni SX - extraction	pH	6	Liu et al. (2019)
Ni SX - extraction	O/A ratio	1:1 vol/vol	Liu et al. (2019)
Ni SX - extraction	D2EHPA in kerosene	25 vol.%	Liu et al. (2019)
Ni SX - extraction	TBP in kerosene	5 vol.%	Liu et al. (2019)
Ni SX - stripping	O/A ratio	1:1 vol/vol	Estimate
Ni SX - stripping	H ₂ SO ₄ concentration	0.1 mol/L	Estimate
Effluent treatment	pH	7	Estimate

S1.4. Power consumption

The power consumption was estimated by dimensioning the largest equipment based on the throughput to the model. The calculated equipment were reactors, thickeners, filters, copper electrowinning, crystallizers, centrifuges, the furnace, and gas cleaning units. The methodology has also been described by Rinne et al. (2021) and Elomaa et al. (2020). All equipment aside from electrowinning were calculated with a +20% safety factor.

The energy consumption by pumps, automation systems, fans, and other necessary equipment is challenging to assess with the simulation alone without a specific equipment list. The total power consumption was therefore assumed to be 1.5 times the calculated value for the hydrometallurgical equipment. The smelter power consumption was estimated from the EverBatt model specific for each type of feed (pre-treated or non-pre-treated NMC or LFP materials), assuming 75% of the energy is consumed by the smelter processes.

Reactor power consumption comes from the agitation of the slurry and relates to the agitator geometry, slurry settling properties, and gas dispersion. It was assumed that reactors without gas dispersion consume 0.4 kW/m³, and the aerated leaching reactor consumes 0.6 kW/m³. The residence times in the feed preparation, carbonation, and neutralization units were assumed to be 60 minutes. The dissolution of lithium chloride is rapid and was assumed to occur in 30 minutes. The residence time in alloy leaching was assumed 8 hours (Xiao et al., 2017). Tran et al. (2022) used hydrogen peroxide as an oxidant for the reduction smelted copper-nickel-cobalt alloy, but it was assumed in this study that oxygen sparging would be sufficient, like in the work of Xiao et al. (2017). The mixer-settlers of solvent extraction units consume far less energy: 0.01-0.02 kWh/m³ (Schlesinger et al., 2021). It was assumed that all circuits have two extraction and two stripping stages: altogether four mixer-settlers per SX circuit.

Copper electrowinning is a well-known process, and the average energy consumption is estimated 2 kWh/kg Cu cathode in sulfate solutions. The cathodic reaction is copper deposition, reaction S1, and the anodic reaction is oxygen evolution (S2). The theoretical energy consumption is much lower, 0.75 kWh/kg Cu.



Crystallizers and centrifuges were also estimated with volumetric flow-based constants. Mechanical vapor compression was presumed for the crystallizers, consuming ~10 kWh for 1 m³ condensed vapor (Nafey et al., 2008). The centrifuges were presumed to consume 1 kWh for 1 m³ feed slurry (Szepessy and Thorwid, 2018).

The filters were selected from Metso's filter brochures (2024) by first estimating the needed filter area using a dry solids rate, which can vary as much as 25-250 kg/m²h (Svarovsky, 2000). The type of filter and performance depends on the filtration characteristics of the residues, which must be determined experimentally. As a rule, amorphous and gel-like precipitates, such as silica gels, aluminum hydroxides, and iron residues are challenging to filter, while crystalline solids filter more readily. The residues and products from lithium flue dust processing (lithium carbonate, calcium carbonate, and calcium fluoride) were all assumed to be easy to filter and were estimated with 200 kg/m²h solids rate, while the alloy leaching and hydroxide filters were estimated with 75 kWh/m²h.

Thickeners were estimated with the procedure first presented by Elomaa et al. (2020). The power consumption by the thickener rake motor was calculated with eq. (S3).

$$P(\text{kW}) = \frac{2\pi NT}{E \cdot 1000 \cdot 60 \text{ s/min}} \quad (\text{S3})$$

Where P is power (kW), N is rotation speed (rpm), T is trip torque (Nm), and E is efficiency (50%).

Trip torque was calculated with eq. (S4). The duty factor K depends on slurry and thickener properties, and examples have been collected by Elomaa et al. (2020). Most mineral processing operations would fall in the “heavy-duty” category, where the duty factor ranges from 10-35 lbs/ft, or ~15-50 N/m, and 30 N/m was used in the calculations.

$$T(\text{Nm}) = KD^2 \quad (\text{S4})$$

Where K is duty factor (N/m), and D is thickener diameter (m).

Rotation speed N (in rpm) was obtained from thickener geometry by assuming that the rake tip speed is 8 m/min. The diameter for rotation speed and eq. S4 can be calculated from thickener area A, given by eq. S5. The necessary liquid/solid ratios, solid feed rate, and liquid specific gravity can be directly taken from the simulation. The settling rate of particles was estimated as 100 mm/h.

$$A(\text{m}^2) = \frac{(F-D)W}{RS} \quad (\text{S5})$$

Where F is the liquid/solid ratio (by weight) at inlet, D is the liquid/solid ratio at outlet, W is the rate at which solids are fed to the thickener (kg/s), R is the settling rate of solids (m/s), and S is the specific gravity of the liquid (kg/m³).

Although the procedure for thickener estimation contains a lot of assumptions and averages, the rake motor consumption is typically very low even for very large heavy-duty thickeners. The assumptions should therefore not affect the overall power consumption let alone the environmental impacts very significantly.

S1.5. Recovery efficiencies

The recoveries of both individual elements and battery weight were estimated with the simulation to assess whether the EU Battery Regulation 2030 targets can be reached: 70% battery weight, 70% lithium, and 95% cobalt, copper, and nickel. It is not completely clear how the “battery weight” is determined in the Regulation given that the calculation methodology has not been established at the time of writing this (European Commission, 2030). The methodology used in this study is based on the current draft.

The calculation of the recovery of individual elements is straightforward, and determined as follows by **Eq. S6**. The recoveries were determined for the whole system boundary, with or without pre-treatment. The recovery of active materials in pre-treatment was assumed 95%, and the recovery of current collector metals 90%.

$$rMe(\text{wt. \%}) = 100 \cdot \frac{\sum m_{Me,\text{output}}}{m_{Me,\text{input}}} \quad (\text{S6})$$

Where rMe is the recovery of an individual metal (Li, Ni, Co, Cu, Al) in the process (%), $m_{Me,\text{output}}$ is the recovered mass of the metal, i.e., metal that is not incorporated in slags or residues (kg), and $m_{Me,\text{input}}$ is the mass of the metal in the input fraction.

For lithium, the input fraction also includes the lithium bound in the electrolyte salt, LiPF₆, as determined in the draft (European Commission, 2030). In terms of copper and aluminum, the recovery was also determined at cell level, although pack materials such as casings and electronics may contain these metals. The copper and aluminum were therefore solely from the current collectors.

The interpretation of “battery weight” is more challenging, but the draft specifies that the “input fraction” refers to all pack materials. The following are included by the draft and necessary for the calculations:

- Dry mass of water-based fluids and acids
- Mass of waste battery casing
- Cables, excluding the ones required to connect the battery to the final equipment
- External parts included in the battery, such as printed circuit boards

It is also stated that “oxygen, carbon at cell level, iron at cell level, phosphorus, chlorine, and sulfur may be taken into account in calculating recycling efficiency in the input and output fractions”, which indicates that carbonaceous materials (i.e., graphite) should be considered together with the organics in the electrolyte. Cathode oxygen was excluded from both the “input” and “output” fractions for simplicity: the recovered lithium, nickel, and cobalt salts contain oxygen, but oxygen is not “recovered” in the process. The mass of electrolyte, plastics, and polymers was included with oxygen.

It was assumed that cell mass comprises 60% of whole battery weight, and the rest (40%) of the materials are recovered at 100% efficiency. This gives an upper limit for the weight recovery efficiency, given by **Eq. S7**.

$$re(\text{wt. \%}) = 100 \cdot 0.6 \cdot \frac{\sum m_{\text{output,cell}}}{m_{\text{input,cell}}} + 0.4 \cdot re_{\text{pack materials}} \quad (\text{S7})$$

where re is weight recovery efficiency (wt.%), $\sum m_{\text{output,cell}}$ is the total mass of recovered materials without cathode oxygen, and $m_{\text{input,cell}}$ is the mass of the input cells (cathode without oxygen, graphite, electrolyte, plastics and polymers), and $re_{\text{pack materials}}$ is the recovery efficiency of pack materials, 100%.

S2. Detailed life cycle inventories

The datasets and more specific unit process are provided in the following sections.

S2.1. Electricity modeling

The forecast for EU's electricity production was obtained from the European Commission's reference scenario 2020 for the year 2030, **Table S3** (De Vita et al., 2021), predicting that 76% of electricity will be sourced from renewables or nuclear fission. The source may be outdated as it assumes that natural gas will be used as a transition fuel, which is uncertain. The regional choices background data from ecoinvent 3.10 were made based on the size of the economies: Germany being overall the largest, but France the most significant producer of nuclear power.

Table S3. The used electricity mix for 2030, adapted from De Vita et al. (2021)

Power source and database item	% MJ
Wind power <i>DE: electricity production, wind, <1 MW turbine, onshore</i>	30
Hydropower <i>DE: electricity production, hydro, run-of-river</i>	12
Solar power <i>DE: electricity production, photovoltaic, 570 kWp open ground installation, multi-Si</i>	12
Biomass <i>GLO: electricity production, wood, future</i>	5
Hard coal <i>DE: electricity production, hard coal</i>	8
Natural gas <i>DE: electricity production, natural gas, conventional power plant</i>	15
Oil <i>DE: electricity production, oil</i>	1
Nuclear power <i>FR: electricity production, nuclear, pressure water reactor</i>	17

S2.2. Process steps

The LCI for grouped unit processes are provided in Tables **S4-S6**. Indicator flows are marked inside brackets, and background data under the flow with *italic*. Products are highlighted by **bold**.

Table S4. Life cycle inventories for the pre-treatment step, modified from EverBatt tool (Dai et al., 2019). The FU is 1000 kg cells.

Flow	<i>dp-111</i>	<i>dp-811</i>	<i>dp-LFP</i>	<i>pt-111</i>	<i>pt-811</i>	<i>pt-LFP</i>	Unit
In: Cells (waste, no burdens)	1000	1000	1000	1000	1000	1000	kg/FU
In: Nitrogen, liquid <i>PER: market for nitrogen, liquid</i>	-	-	-	50.00	50.00	50.00	kg/FU
In: Lime <i>Europe w/o Switzerland: market for lime, packed</i>	-	-	-	36.54	36.61	39.36	kg/FU
In: Diesel <i>GLO: market for diesel, burned in diesel-electric generating set, 10 MW</i>	-	-	-	600	600	600	MJ/FU
In: Natural gas <i>Europe w/o Switzerland: market for heat, district or industrial, natural gas</i>	-	-	-	2000	2000	2000	MJ/FU
In: Electricity <i>Modeled according to section S2.1</i>	-	-	-	200	200	200	MJ/FU
In: Process water <i>PER: market group for tap water</i>	-	-	-	0.38	0.38	0.38	m ³ /FU
Intermediate: Black mass (mass-based flow)	-	-	-	699.11	699.63	665.35	kg/FU
Product: Aluminum scrap <i>IAI Area, EU27 & EFTA: market for aluminium, primary, ingot</i>	-	-	-	46.73	46.37	53.31	kg/FU
Product: Copper metal <i>GLO: market for copper, cathode</i>	-	-	-	72.63	70.16	86.68	kg/FU
Waste: Flue dust (blast furnace dust)	-	-	-	0.90	0.89	0.97	kg/FU
Waste: Solid waste (average incineration residue)	-	-	-	173.29	175.72	185.54	kg/FU
Waste: Wastewater (wastewater, average)	-	-	-	378.54	378.54	378.54	kg/FU
Emissions: Carbon dioxide (carbon dioxide, fossil)	-	-	-	201.00	203.00	223.00	kg/FU

Table S5. LCI for the pyrometallurgical processing and gas cleaning units, per 1 tonne of cells. Note the units.

	<i>dp-111</i>	<i>dp-811</i>	<i>dp-LFP</i>	<i>pt-111</i>	<i>pt-811</i>	<i>pt-LFP</i>	Unit/FU
Pyrometallurgical processing and gas cleaning							
In: Limestone <i>RoW: market for limestone, crushed, washed</i>	503.16	252.31	1893.11	132.88	0.00	1370.22	kg
In: Quartz sand <i>GLO: market for silica sand</i>	670.04	491.76	1859.51	351.69	268.02	1376.85	kg
In: Air, pressurized <i>PER: market for compressed air, 700 kPa gauge</i>	3924.66 481.40	4277.52 524.71	10,904.80 1337.83	2806.09 344.24	3197.51 392.27	4663.75 572.18	kg m ³
In: Recycled slag <i>RoW: market for granulated blast furnace slag</i>	0	411.94	929.75	67.95	531.66	688.42	kg
In: Calcium chloride <i>PER: market for calcium chloride</i>	326.12	301.12	200.89	305.47	278.62	183.07	kg
In: Lime (CaO) <i>Europe w/o Switzerland: market for lime, packed</i>	64.17	62.44	53.16	31.23	28.49	18.90	kg
In: Electricity <i>Modeled according to section S2.1</i>	810.00	795.00	892.5	405.00	405.00	412.50	MJ
In: Natural gas <i>Europe w/o Switzerland, market for heat, district or industrial, natural gas</i>	4604.07	4932.78	12,946.93	3252.72	3638.23	51.32	MJ
In: Coke <i>GLO: market for coke</i>	0 0	0 0	376.33 21,074.48	0 0	0 0	144.31 8081.36	kg MJ
In: Cooling water <i>PER: market group for tap water</i>	5054.05	5746.00	5848.01	3771.32	4193.24	3316.85	kg
Waste: Slag (GLO: copper slag)	1340.09	1312.85	4462.86	954.34	959.37	3304.48	kg
Waste: Heat losses (Not mapped in the LCIA)	508.62	458.22	3048.36	269.86	312.86	849.58	MJ
Emissions to air: Carbon dioxide (carbon dioxide, fossil)	1397.13	1410.77	2691.87	988.43	1045.07	1950.18	kg
Emissions to air: Dust (Particulates >2.5 um, and <10 um)	0.06	0.05	0.04	0.05	0.04	0.03	kg

Lithium recovery by dust refining							
In: Electricity <i>Modeled according to section S2.1</i>	36.19	35.97	35.05	26.45	26.22	24.10	MJ
In: Steam <i>PER: market for steam, in chemical industry</i>	108.00	101.64	74.12	85.53	77.95	51.32	MJ
In: Process water <i>PER: market group for tap water</i>	1271.30	1202.80	866.18	1041.93	946.46	621.55	kg
In: Soda <i>GLO: market for soda ash, dense</i>	298.62	275.48	183.21	281.06	256.31	168.41	kg
Product: Lithium carbonate <i>GLO: market for lithium carbonate</i>	165.23	152.38	101.22	155.66	141.95	93.27	kg
Waste: Solid residues (fluorspar, 97% purity)	102.10	98.72	81.87	55.46	50.58	33.49	kg
Waste: Wastewater (wastewater, average)	1686.23	1586.01	1123.92	1431.76	1302.45	856.69	kg
Aqueous emissions: Fluoride to freshwater (Fluoride)	0.02	0.02	0.02	0.02	0.01	0.01	kg
Aqueous emissions: Chloride to freshwater (Chloride)	208.32	192.36	128.33	195.13	177.98	116.95	kg

Table S6. LCI for the hydrometallurgical alloy refining process, per 1 tonne of cells. Note the units.

	<i>dp-111</i>	<i>dp-811</i>	<i>dp-LFP</i>	<i>pt-111</i>	<i>pt-811</i>	<i>pt-LFP</i>	Unit
Hydrometallurgical processing of alloy							
In: Electricity <i>Modeled according to section S2.1</i>	930.64	949.92	290.39	292.80	324.53	15.07	MJ
In: Steam <i>PER: market for heat, from steam, in chemical industry</i>	4514.39	5229.61	0.00	3137.12	3518.57	0.00	MJ
In: Process water <i>PER: market group for tap water</i>	8644.20	10356.68	1817.68	6152.16	7538.29	108.63	kg
In: Oxygen <i>PER: market for oxygen, liquid</i>	229.26	277.81	79.10	162.14	206.26	3.94	kg

In: Sulfuric acid <i>PER: market for sulfuric acid</i>	1130.48	1295.88	471.53	721.57	880.11	0.00	kg
In: Caustic soda <i>GLO: market for sodium hydroxide, w/o water, in 50% solution state</i>	636.16	712.52	340.54	579.02	696.02	52.18	kg
In: Lime (CaO) <i>Europe w/o Switzerland: market for lime, packed</i>	20.33	39.70	6.80	22.71	28.33	0.34	kg
In: Kerosene <i>Europe w/o Switzerland: market for kerosene</i>	405.93	473.77	113.47	282.00	342.67	7.51	kg
In: Extractants <i>GLO: market for chemical, organic</i>	175.84	205.79	75.65	121.19	148.48	5.01	kg
Product: Copper cathode <i>GLO: market for copper, cathode</i>	76.10	73.51	90.80	3.84	3.71	4.64	kg
Product: Cobalt sulfate (as CoSO ₄) <i>ROW: market for cobalt sulfate</i>	230.28	63.90	-	218.40	60.15	-	kg
Product: Nickel sulfate (as NiSO ₄) <i>GLO: market for nickel sulfate</i>	235.32	531.42	-	224.88	506.34	-	kg
Waste: Solid residues (leach residue from copper production)	71.63	155.09	26.38	88.62	110.56	1.24	kg
Waste: Wastewater (wastewater, average)	6012.03	7163.75	2652.51	4187.34	5161.60	157.88	kg
Aqueous emissions: Copper to water (Copper)	15.48	16.39	18.20	0.70	0.68	0.79	g
Aqueous emissions: Cobalt to water (Cobalt)	10.04	3.06	-	10.61	2.96	-	g
Aqueous emissions: Nickel to water (Nickel, ion)	36.02	53.12	-	28.79	44.00	-	g
Aqueous emissions: Manganese to water (Manganese)	52.83	65.15	-	37.56	47.76	-	g

S2.3. Sensitivity analysis

The re-calculated compositions for the sensitivity analysis are provided in **Table S7**. They were obtained from a mass balance assuming that either half or 90% of graphite is removed in the pre-treatment stage.

Table S7. Compositions of the black masses for the sensitivity analysis.

	Low graphite black mass (Low, “L”)		
	NMC111	NMC811	LFP
Black mass (kg/t cells)	452.23	417.74	444.12
LiCoO ₂ (wt.%)	32.80	9.90	0.00
LiNiO ₂ (wt.%)	32.72	79.03	0.00
LiMnO ₂ (wt.%)	32.29	8.66	0.00
LiFePO ₄ (wt.%)	0.00	0.00	97.60
Carbon (wt.%)	0.55	0.68	0.50
Aluminum (wt.%)	0.57	0.62	0.67
Copper (wt.%)	0.90	0.94	1.08
LiPF ₆ (wt.%)	0.00	0.00	0.00
PVDF (wt.%)	0.17	0.17	0.15

The inventories for the sensitivity analyses are given in **Table S8**. Graphite was not credited as a product, nor was it provided any downstream refining process.

Table S8. LCI for the sensitivity analysis, FU = 1 tonne of cells.

Inflows	L-III	L-8II	L-LFP	Unit/FU
Cells	1.00	1.00	1.00	t
Electricity	1117.68	1150.94	802.02	MJ
Diesel	600.00	600.00	600.00	MJ
Heat, natural gas	8829.86	8792.45	9804.12	MJ
Heat, steam	3163.51	3871.17	51.47	MJ
Metallurgical coke	0.10 5338.67	0.10 5436.65	0.26 14,326.58	t MJ
Air, compressed	7.00 858.77	7.00 858.77	7.43 913.00	t m ³
Oxygen, liquid	0.16	0.21	0.00	t
Nitrogen, liquid	0.05	0.05	0.05	t
Water	11.29	12.54	1.24	t
Silica sand	0.35	0.27	1.13	t
Limestone (CaCO ₃)	0.13	0.00	1.18	t
Blast furnace slag	0.07	0.53	0	t
Calcium chloride	0.31	0.28	0.18	t
Lime (CaO)	0.09	0.09	0.06	t
Soda ash	0.28	0.26	0.17	t
Sulfuric acid	0.69	0.85	0.00	t
Caustic soda	0.58	0.70	0.08	t
Kerosene	0.28	0.34	0.01	t
Organic chemicals	0.12	0.15	0.06	t
Outflows	L-III	L-8II	L-LFP	Unit/FU
Product: Aluminum	46.73	46.37	53.31	kg
Product: Copper scrap	72.63	70.16	86.68	kg
Product: Copper cathode	3.85	3.72	4.54	kg
Product: Cobalt sulfate	218.43	61.85	0	kg
Product: Nickel sulfate	225.10	506.95	0	kg
Product: Lithium carbonate	155.56	142.14	93.15	kg
Waste: Solid slag	0.75	0.96	2.27	t
Waste: Wastewater	5.99	6.84	4.96	t
Waste: Solid residues	0.32	0.34	0.36	t
Emissions: PM (>2.5 um, <10 um)	0.04	0.04	0.03	kg
Emissions: Carbon dioxide to air	0.62	0.37	4.96	t
Emissions: Fluoride to freshwater	0.02	0.02	0.01	kg
Emissions: Chloride to freshwater	195.08	178.21	116.88	kg
Emissions: Copper to freshwater	0.73	0.64	0.69	g
Emissions: Nickel to freshwater	28.72	44.11	0	g
Emissions: Cobalt to freshwater	10.62	2.96	0	g

S3. Tabulated results

S3.1. Recoveries from simulation

The recoveries for individual materials and total cell mass are provided in **Table S9**. The differences between respective *dp* and *pt* scenarios are mainly due to the cathode losses and recovered metals in pre-treatment. The “*L*” scenarios refer to the low graphite black masses used in the sensitivity analyses, and the cell mass was calculated with 90% graphite recovery to assess the effect on total pack material recovery, but graphite was not considered in the LCA stage. The total pack mass calculated on the Table assumes that pack materials, such as the management system and casing, account for 40% of the battery weight, and 100% is recovered. The value is therefore only a theoretical maximum.

The recovered copper is marked as “total” since it includes both the mechanically separated copper in the *pt* scenarios and the hydrometallurgically electrowon copper.

Table S9. Material recoveries (wt.%) from the cells.

	<i>dp-111</i>	<i>dp-811</i>	<i>dp-LFP</i>	<i>pt-111</i>	<i>pt-811</i>	<i>pt-LFP</i>	<i>L-111</i>	<i>L-811</i>	<i>L-LFP</i>
Total cell weight*	35.5	38.6	13.3	39.7	42.6	19.9	66.2	73.6	45.7
Total battery weight*	61.3	63.2	48.0	63.8	65.6	51.9	79.8	84.2	67.4
Copper (total)	94.3	94.2	93.6	94.6	95.0	93.7	94.8	94.7	94.7
Aluminum	0	0	0	90.0	90.0	90.0	90.0	90.0	90.0
Lithium	91.3	91.2	90.8	86.0	85.0	91.8	87.9	87.3	82.0
Cobalt	93.1	92.8	-	88.3	87.3	-	88.3	89.8	0
Nickel	95.3	96.5	-	91.1	92.0	-	91.2	92.1	0

* Cathode mass calculated without oxygen, *L* scenarios calculated assuming 90% graphite may be recovered

S3.2. Impact assessment

Table S10. Results of the impact assessment (per 1 tonne of cells), “PT” refers to pre-treatment.

	dp-111									
	PT	Pyro	Alloy refining	Dust refining	Credit, Al	Credit, Cu	Credit, CoSO ₄	Credit, NiSO ₄	Credit, Li ₂ CO ₃	
AP (mol H ⁺ eq)	0	3.89	23.27	1.96	0	-42.34	-60.15	-27.09	-11.79	
GWP (kg CO ₂ eq)	0	2150	2175	395	0	-509	-5550	-1132	-1286	
EP freshwater (kg P eq)	0	0.20	0.72	0.11	0	-3.33	-2.18	-0.41	-0.76	
EP marine (kg N eq)	0	0.62	2.12	1.20	0	-2.02	-8.34	-1.96	-5.17	
EP terrestrial (mol N eq)	0	10.70	21.68	4.51	0	-28.30	-56.40	-14.10	-23.13	
HTP cancer (CTUh)	0	4.19E-7	1.41E-6	3.39E-7	0	-7.68E-6	-1.39E-4	-3.11E-5	-9.13E-7	
HTP non-cancer (CTUh)	0	1.12E-5	3.33E-5	6.55E-6	0	-5.64E-4	-4.89E-4	-1.05E-4	-0.38E-4	
ODP (kg CFC-11 eq)	0	8.28E-5	9.68E-4	2.19E-5	0	-0.28E-4	-7.98E-4	-1.51E-4	-1.38E-4	
POCP (kg NMVOC eq)	0	1.69	7.71	0.98	0	-7.81	-18.50	-5.47	-5.48	
ADP (kg Sb eq)	0	9.81E-3	22.50E-3	6.98E-3	0	-1.02	-1.20	-0.27	-0.04	
	dp-811									
	PT	Pyro	Alloy refining	Dust refining	Credit, Al	Credit, Cu	Credit, CoSO ₄	Credit, NiSO ₄	Credit, Li ₂ CO ₃	
AP (mol H ⁺ eq)	0	3.09	26.67	1.81	0	-40.90	-16.69	-61.18	-10.87	
GWP (kg CO ₂ eq)	0	1940	2489	365	0	-492	-1540	-2557	-1186	
EP freshwater (kg P eq)	0	0.14	0.83	0.11	0	-3.22	-0.61	-1.16	-0.70	
EP marine (kg N eq)	0	0.45	2.43	1.10	0	-1.95	-2.31	-4.44	-4.77	
EP terrestrial (mol N eq)	0	8.47	24.80	4.16	0	-27.29	-15.65	-31.95	-21.33	
HTP cancer (CTUh)	0	3.03E-7	1.61E-6	3.12E-7	0	-7.42E-6	-3.85E-5	-7.02E-5	-8.42E-7	
HTP non-cancer (CTUh)	0	8.5E-6	3.78E-5	0.61E-5	0	-5.45E-4	-1.36E-4	-2.38E-4	-0.35E-4	
ODP (kg CFC-11 eq)	0	5.08E-5	1.11E-3	2.03E-5	0	-0.27E-4	-2.21E-4	-3.40E-4	-1.27E-4	
POCP (kg NMVOC eq)	0	1.19	8.85	0.91	0	-7.54	-5.13	-12.35	-5.05	
ADP (kg Sb eq)	0	8.15E-3	-2.56E-2	6.44E-3	0	-0.99	-0.33	-0.62	-0.04	

<i>dp-LFP</i>									
	PT	Pyro	Alloy refining	Dust refining	Credit, Al	Credit, Cu	Credit, CoSO₄	Credit, NiSO₄	Credit, Li₂CO₃
AP (mol H ⁺ eq)	0	7.64	9.22	1.21	0	-50.52	0.00	0.00	-7.22
GWP (kg CO ₂ eq)	0	4300	768	244	0	-607	0.00	0.00	-788
EP freshwater (kg P eq)	0	0.99	0.32	0.07	0	-3.98	0.00	0.00	-0.47
EP marine (kg N eq)	0	1.53	0.86	0.74	0	-2.41	0.00	0.00	-3.17
EP terrestrial (mol N eq)	0	17.80	8.61	2.78	0	-33.71	0.00	0.00	-14.17
HTP cancer (CTUh)	0	1.71E-5	5.91E-7	2.08E-7	0	-9.16E-6	0.00	0.00	-5.59E-7
HTP non-cancer (CTUh)	0	2.36E-5	1.48E-5	4.03E-6	0	-6.73E-4	0.00	0.00	-0.23E-4
ODP (kg CFC-11 eq)	0	2.12E-4	3.87E-4	1.36E-5	0	-0.33E-4	0.00	0.00	-8.45E-5
POCP (kg NMVOC eq)	0	11.00	2.99	0.61	0	-9.32	0.00	0.00	-3.36
ADP (kg Sb eq)	0	7.35E-3	1.06E-2	4.29E-3	0	-1.22	0.00	0.00	-0.02
<i>pt-III</i>									
	PT	Pyro	Alloy refining	Dust refining	Credit, Al	Credit, Cu	Credit, CoSO₄	Credit, NiSO₄	Credit, Li₂CO₃
AP (mol H ⁺ eq)	0.95	2.79	16.45	1.84	-3.33	-42.55	-57.00	-25.90	-11.10
GWP (kg CO ₂ eq)	383	1380	1660	370	-457	-511	-5260	-1080	-1210
EP freshwater (kg P eq)	0.02	0.12	0.58	0.11	-0.20	-3.35	-2.07	-0.49	-0.72
EP marine (kg N eq)	0.38	0.36	1.66	1.13	-0.45	-2.03	-7.91	-1.88	-4.87
EP terrestrial (mol N eq)	4.17	7.65	16.87	4.23	-4.51	-28.43	-53.50	-13.50	-21.80
HTP cancer (CTUh)	2.37E-8	2.69E-7	1.07E-6	3.18E-7	-1.14E-6	-7.72E-6	-1.32E-4	-2.97E-5	-8.60E-7
HTP non-cancer (CTUh)	9.50E-7	7.81E-6	2.64E-5	6.16E-6	-0.17E-5	-5.67E-4	-4.64E-4	-1.01E-4	-0.38E-4
ODP (kg CFC-11 eq)	2.94E-5	4.18E-5	7.77E-4	2.03E-5	-0.34E-5	-0.28E-4	-7.57E-4	-1.44E-4	-1.30E-4
POCP (kg NMVOC eq)	1.12	0.93	5.79	0.92	-1.49	-7.84	-17.55	-5.23	-5.16
ADP (kg Sb eq)	1.65E-4	7.88E-3	1.76E-2	6.56E-3	-0.82E-3	-1.03	-1.14	-0.26	-0.04

pt-811									
	PT	Pyro	Alloy refining	Dust refining	Credit, Al	Credit, Cu	Credit, CoSO ₄	Credit, NiSO ₄	Credit, Li ₂ CO ₃
AP (mol H ⁺ eq)	0.95	2.65	19.89	1.68	-3.31	-41.10	-15.71	-58.29	-10.13
GWP (kg CO ₂ eq)	385	1455	1983	337	-454	-494	-1450	-2436	-1105
EP freshwater (kg P eq)	0.02	0.12	0.70	0.10	-0.20	-3.24	-0.57	-1.10	-0.66
EP marine (kg N eq)	0.38	0.36	1.99	1.03	-0.45	-1.96	-2.18	-4.23	-4.45
EP terrestrial (mol N eq)	4.16	7.31	20.28	3.86	-4.48	-26.05	-14.74	-30.45	-19.87
HTP cancer (CTUh)	2.37E-8	2.58E-7	1.29E-6	2.90E-7	-1.13E-6	-7.46E-6	-3.63E-5	-6.69E-5	-7.85E-7
HTP non-cancer (CTUh)	9.50E-7	7.41E-6	3.18E-5	5.62E-6	-0.17E-4	-5.47E-4	-1.28E-4	-2.27E-4	-0.32E-4
ODP (kg CFC-11 eq)	2.94E-5	4.61E-5	9.34E-4	2.94E-5	-0.34E-4	-0.27E-4	-2.08E-4	-3.24E-4	-1.19E-4
POCP (kg NMVOC eq)	1.12	0.95	6.98	0.84	-1.48	-7.58	-4.83	-11.77	-4.71
ADP (kg Sb eq)	1.65E-4	7.33E-3	2.13E-2	5.99E-3	-0.82E-3	-0.99	-0.31	-0.59	-0.04
pt-LFP									
	PT	Pyro	Alloy refining	Dust refining	Credit, Al	Credit, Cu	Credit, CoSO ₄	Credit, NiSO ₄	Credit, Li ₂ CO ₃
AP (mol H ⁺ eq)	0.95	3.84	0.49	1.10	-3.80	-50.81	0.00	0.00	-6.65
GWP (kg CO ₂ eq)	405	2420	85	222	-522	-611	0.00	0.00	-726
EP freshwater (kg P eq)	0.02	0.42	0.04	0.06	-0.23	-4.00	0.00	0.00	-0.43
EP marine (kg N eq)	0.38	0.70	0.10	0.67	-0.52	-2.42	0.00	0.00	-2.92
EP terrestrial (mol N eq)	4.17	9.34	0.96	2.54	-5.15	-33.91	0.00	0.00	-13.06
HTP cancer (CTUh)	2.38E-8	6.65E-6	5.75E-8	1.91E-7	-1.30E-6	-9.22E-6	0.00	0.00	-5.16E-7
HTP non-cancer (CTUh)	9.51E-7	1.17E-5	1.63E-6	3.69E-6	-0.19E-4	-6.77E-4	0.00	0.00	-0.21E-4
ODP (kg CFC-11 eq)	2.94E-5	5.11E-5	4.85E-5	1.22E-5	-0.39E-4	-0.33E-4	0.00	0.00	-0.78E-4
POCP (kg NMVOC eq)	1.12	4.45	0.28	0.55	-1.70	-9.37	0.00	0.00	-3.09
ADP (kg Sb eq)	1.66E-04	5.46E-3	1.04E-3	3.94E-3	-0.94E-3	-1.23	0.00	0.00	-0.02

S3.3. Contribution analysis

Table S11. Contribution analyses of the *dp* scenarios (% of total process impact.) “Alloy” refers to hydrometallurgical copper-nickel-cobalt refining and “Dust” to lithium recovery from flue dust.

dp-III													
Pyro:	Total	Electricity	Lime	Coke	Silica	Direct	Calcium chloride	Air	Natural gas	Water	BF slag	Limestone	
AP	13.36	2.63	0.06	0	0.79	0.00	8.35	0.61	0.77	0.03	0	0.13	
ADP	24.94	3.43	0.02	0	0.17	0.00	19.87	1.19	0.02	0.02	0	0.03	
GWP	45.55	6.04	0.07	0	0.62	29.66	3.43	0.65	5.06	0.04	0	0.06	
EP freshw.	19.28	6.51	0.14	0	0.52	0.00	8.73	2.95	0.27	0.12	0	0.03	
EP marine	15.81	5.02	0.12	0	1.46	0.00	6.42	0.74	1.64	0.05	0	0.33	
EP terrestre.	29.00	5.64	0.13	0	1.64	0.00	18.38	0.70	1.90	0.05	0	0.47	
HTP canc.	19.35	5.77	0.12	0	0.64	0.00	10.58	0.94	0.89	0.32	0	0.07	
HTP non-c.	21.94	5.48	0.06	0	0.60	0.00	14.02	1.12	0.45	0.20	0	0.08	
ODP	7.72	2.83	0.02	0	0.23	0.00	1.01	0.14	3.42	0.01	0	0.05	
POCP	16.28	5.46	0.12	0	1.66	0.00	5.56	0.70	2.30	0.05	0	0.39	
Alloy:	Total	Electricity	Direct	Kerosene	Lime	Extractant	Caustic soda	Steam	Oxygen	Sulfuric acid	Water		
AP	79.90	0.53	0.00	8.48	0.02	5.49	16.28	5.32	2.35	41.37	0.05		
ADP	57.31	0.69	0.00	0.67	0.01	6.10	29.75	0.41	0.83	18.82	0.04		
GWP	46.08	1.22	0.00	4.22	0.02	7.71	17.51	10.05	2.70	2.58	0.06		
EP freshw.	69.67	1.31	0.00	1.51	0.04	6.77	37.67	4.36	12.12	5.70	0.20		
EP marine	53.81	1.01	0.00	7.94	0.04	7.31	24.59	5.68	3.04	4.11	0.08		
EP terrestre.	58.78	1.14	0.00	9.24	0.04	8.27	26.02	6.42	2.85	4.72	0.08		
HTP canc.	65.01	1.17	0.00	4.10	0.04	18.84	24.20	4.76	1.89	9.47	0.55		
HTP non-c.	65.22	1.11	0.00	4.74	0.02	6.33	34.87	3.25	2.68	11.89	0.33		
ODP	90.24	0.57	0.00	31.69	0.01	3.02	46.61	6.32	0.60	1.41	0.02		
POCP	74.25	1.11	0.00	13.39	0.04	12.82	24.67	7.43	2.76	11.95	0.09		
Dust:	Total	Electricity	Soda	Direct	Steam	Water							
AP	6.74	0.02	6.58	0	0.13	0.01							

ADP	17.74	0.03	17.70	0	0.01	0.01							
GWP	8.37	0.05	8.08	0	0.24	0.01							
EP freshw.	11.05	0.05	10.87	0	0.10	0.03							
EP marine	30.38	0.04	30.20	0	0.14	0.01							
EP terrestr.	12.22	0.04	12.01	0	0.15	0.01							
HTP canc.	15.64	0.05	15.39	0	0.11	0.08							
HTP non-c.	12.84	0.04	12.67	0	0.08	0.05							
ODP	2.04	0.02	1.87	0	0.15	0.00							
POCP	9.47	0.04	9.23	0	0.18	0.01							
Credits:	Total	Copper	Aluminum	CoSO₄	NiSO₄	Li₂CO₃							
AP	-485.51	-145.42	0	-206.56	-93.04	-40.49							
ADP	-6435.38	-2593.53	0	-3051.21	-691.61	-99.04							
GWP	-179.58	-10.78	0	-117.57	-23.99	-27.24							
EP freshw.	-654.94	-321.39	0	-210.47	-49.46	-73.62							
EP marine	-443.91	-51.26	0	-211.62	-49.73	-131.30							
EP terrestr.	-330.52	-76.71	0	-152.88	-38.22	-62.71							
HTP canc.	-8252.71	-354.69	0	-6419.53	-1436.31	-42.18							
HTP non-c.	-2342.02	-1104.74	0	-957.84	-205.67	-73.77							
ODP	-359.02	-2.57	0	-74.38	-14.07	-12.86							
POCP	-6435.38	-75.25	0	-178.26	-52.71	-52.80							

dp-811

Pyro:	Total	Electricity	Lime	Coke	Silica	Direct	Calcium chloride	Air	Natural gas	Water	BF slag	Limestone
AP	9.79	0.42	0.05	0	0.53	0	7.13	0.62	0.76	0.03	0.19	0.06
ADP	20.3	0.58	0.02	0	0.12	0	17.98	1.27	0.21	0.02	0.09	0.01
GWP	40.41	1.03	0.06	0	0.45	29.43	3.11	0.69	5.34	0.04	0.23	0.03
EP freshw.	13.05	1.09	0.13	0	0.37	0	7.81	3.12	0.28	0.13	0.11	0.01
EP marine	11.21	0.86	0.12	0	1.06	0	5.88	0.80	1.74	0.05	0.53	0.17
EP terrestr.	22.64	0.96	0.12	0	1.19	0	16.72	0.75	2.01	0.05	0.60	0.24
HTP canc.	13.57	0.97	0.11	0	0.46	0	9.47	1.00	0.92	0.36	0.25	0.03

HTP non-c.	16.22	0.92	0.06	0	0.43	0	12.62	1.19	0.47	0.22	0.27	0.04
ODP	5.12	0.44	0.02	0	0.15	0	0.84	0.14	3.32	0.01	0.18	0.02
POCP	10.91	0.90	0.11	0	1.15	0	4.86	0.72	2.34	0.06	0.59	0.18
Alloy:	Total	Electricity	Direct	Kerosene	Lime	Extractant	Caustic soda	Steam	Oxygen	Sulfuric acid	Water	
AP	84.49	0.50	0	9.12	0.03	5.94	16.81	5.68	2.62	43.73	0.06	
ADP	74.65	0.69	0	0.76	0.01	7.00	32.59	11.46	0.98	21.12	0.04	
GWP	51.98	1.23	0	4.86	0.04	8.88	19.31	11.46	3.22	2.91	0.07	
EP freshw.	77.12	1.29	0	1.71	0.08	7.66	40.77	4.88	14.19	6.31	0.23	
EP marine	61	1.03	0	9.20	0.07	8.49	27.29	6.51	3.65	4.67	0.09	
EP terrestr.	66.24	1.14	0	10.61	0.08	9.52	28.72	7.35	3.39	5.34	0.09	
HTP canc.	72.41	1.16	0.00	4.65	0.07	21.44	26.31	5.38	2.22	10.53	0.65	
HTP non-c.	72.21	1.10	0.00	5.39	0.04	7.22	37.96	3.66	3.16	13.29	0.39	
ODP	93.16	0.53	0	33.41	0.01	3.20	47.25	6.62	0.66	1.46	0.02	
POCP	80.8	1.07	0	14.83	0.07	14.20	26.22	8.16	3.17	12.98	0.10	
Dust:	Total	Electricity	Soda	Direct	Steam	Water						
AP	5.74	0.02	5.60	0	0.11	0.01						
ADP	16.03	0.03	15.99	0	0.01	0.00						
GWP	7.62	0.05	7.34	0	0.22	0.01						
EP freshw.	9.86	0.05	9.69	0	0.09	0.03						
EP marine	27.79	0.04	27.61	0	0.13	0.01						
EP terrestr.	11.11	0.04	10.92	0	0.14	0.01						
HTP canc.	14.02	0.04	13.80	0	0.10	0.08						
HTP non-c.	11.55	0.04	11.39	0	0.07	0.05						
ODP	1.71	0.02	1.56	0	0.13	0.00						
POCP	8.29	0.04	8.08	0	0.16	0.01						
Credits:	Total	Copper	Aluminum	CoSO₄	NiSO₄	Li₂CO₃						
AP	-410.61	-129.51	0	-52.85	-193.72	-34.42						
ADP	-4915.52	-2464.29	0	-831.01	-1530.53	-89.47						
GWP	-120.46	-10.25	0	-32.12	-53.33	-24.73						

EP freshw.	-530.95	-300.01	0	-56.44	-107.94	-65.61							
EP marine	-338.50	-49.00	0	-58.18	-111.58	-120.01							
EP terrestr.	-257.09	-72.93	0	-41.83	-85.39	-57.01							
HTP canc.	-5248.59	-332.88	0	-1729.30	-3149.23	-37.79							
HTP non-c.	-1820.15	-1040.05	0	-259.19	-454.62	-66.31							
ODP	-60.34	-2.25	0	-18.66	-28.70	-10.73							
POCP	-274.94	-68.92	0	-46.89	-112.85	-46.16							

dp-LFP

Pyro:	Total	Electricity	Lime	Coke	Silica	Direct	Calcium chloride	Air	Natural gas	Water	BF slag	Limestone
AP	42.29	0.82	0.08	21.75	3.51	0	8.30	2.75	3.48	0.06	0.75	0.79
ADP	33.03	1.18	0.04	1.96	0.81	0	21.61	5.83	1.01	0.04	0.37	0.18
GWP	80.97	1.04	0.05	10.90	1.53	50.64	1.88	1.60	12.63	0.04	0.46	0.20
EP freshw.	71.82	0.95	0.08	58.57	1.09	0	4.04	6.15	0.56	0.10	0.20	0.08
EP marine	49.13	1.23	0.13	26.04	5.12	0	5.00	2.60	5.83	0.07	1.51	1.60
EP terrestr.	60.85	1.38	0.13	26.00	5.76	0	14.29	2.47	6.75	0.07	1.74	2.26
HTP canc.	95.79	0.14	0.01	93.86	0.22	0	0.79	0.32	0.30	0.05	0.07	0.03
HTP non-c.	55.76	1.28	0.06	35.36	2.00	0	10.40	3.75	1.53	0.27	0.74	0.37
ODP	34.53	0.96	0.03	12.69	1.13	0	1.09	0.69	16.80	0.02	0.80	0.32
POCP	75.48	0.75	0.07	60.92	3.27	0	2.43	1.37	4.60	0.04	1.00	1.03
Alloy:	Total	Electricity	Direct	Kerosene	Lime	Extractant	Caustic soda	Steam	Oxygen	Sulfuric acid	Water	
AP	51.07	0.27	0	3.81	0.01	3.81	14.04	0	1.30	27.81	0.02	
ADP	47.78	0.38	0	0.33	0.00	4.64	28.07	0	0.50	13.85	0.01	
GWP	14.48	0.34	0	1.05	0.01	2.95	8.33	0	0.83	0.96	0.01	
EP freshw.	22.93	0.31	0	0.32	0.01	2.19	15.15	0	3.14	1.78	0.03	
EP marine	27.31	0.40	0	2.81	0.02	3.97	16.61	0	1.32	2.16	0.02	
EP terrestr.	29.57	0.45	0	3.26	0.02	4.49	17.60	0	1.24	2.49	0.02	
HTP canc.	3.30	0.04	0.00	0.14	0.00	0.98	1.57	0	0.08	0.48	0.01	
HTP non-c.	34.86	0.42	0.00	1.59	0.01	3.28	22.40	0	1.11	5.97	0.08	
ODP	63.19	0.31	0	15.49	0.00	2.28	43.71	0	0.36	1.03	0.01	

POCP	20.47	0.25	0	2.66	0.01	3.92	9.40	0	0.68	3.54	0.01	
Dust:	Total	Electricity	Soda	Direct	Steam	Water						
AP	6.69	0.03	6.51	0	0.14	0.01						
ADP	19.24	0.05	19.17	0	0.01	0.01						
GWP	4.60	0.04	4.40	0.00	0.15	0.01						
EP freshw.	5.11	0.04	5.01	0.00	0.05	0.01						
EP marine	23.56	0.05	23.38	0.00	0.12	0.01						
EP terrestr.	9.50	0.05	9.31	0.00	0.13	0.01						
HTP canc.	1.17	0.01	1.14	0.00	0.01	0.01						
HTP non-c.	9.50	0.05	9.35	0.00	0.06	0.04						
ODP	2.22	0.04	2.00	0.00	0.18	0.00						
POCP	4.16	0.03	4.03	0.00	0.09	0.01						
Credits:	Total	Copper	Aluminum	CoSO₄	NiSO₄	Li₂CO₃						
AP	-319.53	-279.57	0	0	0	-39.96						
ADP	-5592.43	-5485.33	0	0	0	-107.09						
GWP	-26.26	-11.43	0	0	0	-14.83						
EP freshw.	-321.91	-288.04	0	0	0	-33.87						
EP marine	-178.61	-77.08	0	0	0	-101.53						
EP terrestr.	-164.05	-115.50	0	0	0	-48.55						
HTP canc.	-54.33	-51.20	0	0	0	-3.13						
HTP non-c.	-1640.55	-1586.17	0	0	0	-54.38						
ODP	-19.16	-5.37	0	0	0	-13.79						
POCP	-86.86	-63.86	0	0	0	-23.00						

Table S12. Contribution analyses of the *pt* scenarios (% total process impacts). “Alloy” refers to hydrometallurgical copper-nickel-cobalt refining and “Dust” to lithium recovery from flue dust.

<i>pt-III</i>												
<i>Pre-treat:</i>	Total	Electricity	Natural gas	Lime	Diesel	Direct	Nitrogen	Water				
AP	4.29	0.15	0.44	0.04	3.38	0.00	0.27	0.00				

ADP	0.51	0.18	0.11	0.02	0.12	0.00	0.09	0.00				
GWP	10.09	0.33	2.73	0.05	1.39	5.30	0.29	0.00				
EP freshw.	2.02	0.36	0.15	0.10	0.08	0.00	1.33	0.01				
EP marine	10.86	0.24	0.80	0.08	9.44	0.00	0.30	0.00				
EP terrestr.	12.66	0.27	0.93	0.08	11.09	0.00	0.28	0.00				
HTP canc.	1.41	0.32	0.50	0.09	0.26	0.00	0.22	0.03				
HTP non-c.	2.30	0.30	0.24	0.05	1.41	0.00	0.29	0.02				
ODP	3.39	0.15	1.84	0.01	1.31	0.00	0.07	0.00				
POCP	12.74	0.28	1.19	0.08	10.89	0.00	0.29	0.00				
<i>Pyro:</i>	Total	Electricity	Lime	Coke	Silica	Direct	Calcium chloride	Air	Natural gas	Water	BF slag	Limestone
AP	12.66	0.31	0.04	0	0.54	0	10.35	0.58	0.72	0.03	0.04	0.05
ADP	24.45	0.37	0.01	0	0.11	0	22.70	1.04	0.17	0.02	0.02	0.01
GWP	36.29	0.66	0.04	0	0.41	26.05	4.01	0.57	4.46	0.03	0.05	0.02
EP freshw.	14.52	0.72	0.08	0	0.35	0	10.32	2.66	0.24	0.11	0.02	0.01
EP marine	10.25	0.49	0.07	0	0.86	0	6.72	0.59	1.29	0.04	0.10	0.10
EP terrestr.	23.24	0.56	0.07	0	0.97	0	19.29	0.56	1.51	0.04	0.11	0.14
HTP canc.	15.97	0.65	0.07	0	0.43	0	12.74	0.87	0.81	0.31	0.05	0.02
HTP non-c.	18.90	0.60	0.04	0	0.39	0	16.23	0.99	0.39	0.18	0.06	0.03
ODP	4.81	0.31	0.01	0	0.15	0	1.16	0.13	2.99	0.01	0.04	0.02
POCP	10.64	0.57	0.07	0	1.03	0	6.16	0.59	1.93	0.05	0.12	0.12
<i>Alloy:</i>	Total	Electricity	Direct	Kerosene	Lime	Extractant	Caustic soda	Steam	Oxygen	Sulfuric acid	Water	
AP	74.70	0.22	0	7.77	0.03	5.00	19.62	4.90	2.19	34.92	0.05	
ADP	54.68	0.27	0	0.57	0.01	5.13	32.98	0.35	0.71	14.64	0.03	
GWP	43.77	0.48	0	3.64	0.03	6.62	19.83	8.70	2.38	2.05	0.05	
EP freshw.	70.45	0.52	0	1.33	0.06	5.88	43.28	3.82	10.81	4.58	0.18	
EP marine	46.99	0.36	0	6.18	0.05	5.64	24.99	4.39	2.40	2.92	0.06	
EP terrestr.	51.25	0.40	0	7.20	0.05	6.38	26.52	5.01	2.25	3.37	0.06	
HTP canc.	63.63	0.47	0.00	3.67	0.05	16.73	28.40	4.28	1.72	7.80	0.51	
HTP non-c.	63.91	0.43	0.00	4.06	0.03	5.39	39.19	2.78	2.34	9.39	0.30	

ODP	89.46	0.22	0	27.16	0.01	2.57	52.43	5.43	0.52	1.11	0.02	
POCP	66.11	0.41	0	11.03	0.05	10.45	26.63	6.12	2.31	9.03	0.08	
Dust:	Total	Electricity	Soda	Direct	Steam	Water						
AP	8.34	0.02	8.17	0.00	0.13	0.01						
ADP	20.36	0.02	20.32	0.00	0.01	0.01						
GWP	9.75	0.04	9.46	0.00	0.24	0.01						
EP freshw.	13.07	0.05	12.89	0.00	0.10	0.03						
EP marine	31.90	0.03	31.73	0.00	0.12	0.01						
EP terrest.	12.85	0.04	12.67	0.00	0.14	0.01						
HTP canc.	18.94	0.04	18.69	0.00	0.12	0.09						
HTP non-c.	14.90	0.04	14.73	0.00	0.08	0.05						
ODP	2.34	0.02	2.16	0.00	0.15	0.00						
POCP	10.51	0.04	10.30	0.00	0.17	0.01						
Credits:	Total	Copper	Aluminum	CoSO₄	NiSO₄	Li₂CO₃						
AP	-635.26	-193.25	-15.13	-258.85	-117.62	-50.41						
ADP	-7652.77	-3193.25	-2.56	-3536.69	-806.47	-113.80						
GWP	-224.59	-13.48	-12.06	-138.67	-28.47	-31.90						
EP freshw.	-830.03	-406.99	-24.31	-251.63	-59.57	-87.52						
EP marine	-485.76	-57.58	-12.81	-224.12	-53.27	-137.99						
EP terrest.	-369.84	-86.37	-13.70	-162.53	-41.01	-66.23						
HTP canc.	-10205.66	-459.50	-67.87	-7858.85	-1768.24	-51.20						
HTP non-c.	-2864.07	-1370.47	-40.88	-1122.50	-244.34	-85.88						
ODP	-125.77	-3.19	-3.94	-87.11	-16.58	-14.96						
POCP	-425.44	-89.54	-17.01	-200.28	-59.68	-58.92						

pt-811

Pre-treat:	Total	Electricity	Natural gas	Lime	Diesel	Direct	Nitrogen	Water				
AP	3.76	0.13	0.39	0.04	2.96	0.00	0.24	0.00				
ADP	0.47	0.17	0.10	0.02	0.11	0.00	0.08	0.00				
GWP	9.25	0.30	2.49	0.04	1.27	4.88	0.27	0.00				

EP freshw.	1.78	0.31	0.13	0.09	0.07	0.00	1.17	0.01				
EP marine	10.17	0.23	0.75	0.07	8.84	0.00	0.28	0.00				
EP terrestr.	11.69	0.25	0.86	0.08	10.24	0.00	0.26	0.00				
HTP canc.	1.27	0.29	0.45	0.08	0.23	0.00	0.19	0.03				
HTP non-c.	2.07	0.27	0.22	0.04	1.27	0.00	0.26	0.02				
ODP	2.86	0.13	1.55	0.01	1.11	0.00	0.06	0.00				
POCP	11.29	0.25	1.05	0.07	9.65	0.00	0.26	0.00				
Pyro:	Total	Electricity	Lime	Coke	Silica	Direct	Calcium chloride	Air	Natural gas	Water	BF slag	Limestone
AP	10.55	0.27	0.03	0	0.36	0.00	8.26	0.58	0.03	0.31	0.03	0
ADP	21.05	0.34	0.01	0	0.07	0.00	19.20	1.09	0.02	0.13	0.01	0
GWP	34.98	0.60	0.03	0	0.28	25.24	3.32	0.60	0.03	0.34	0.03	0
EP freshw.	12.42	0.64	0.07	0	0.23	0.00	8.30	2.67	0.11	0.17	0.07	0
EP marine	9.61	0.46	0.06	0	0.61	0.00	5.73	0.63	0.04	0.72	0.06	0
EP terrestr.	20.52	0.51	0.06	0	0.68	0.00	16.26	0.59	0.04	0.81	0.06	0
HTP canc.	13.88	0.59	0.06	0	0.30	0.00	10.53	0.89	0.31	0.38	0.06	0
HTP non-c.	16.19	0.54	0.03	0	0.27	0.00	13.37	1.02	0.18	0.39	0.03	0
ODP	4.48	0.26	0.01	0	0.10	0.00	0.90	0.12	0.01	0.27	0.01	0
POCP	9.64	0.50	0.06	0	0.70	0.00	4.99	0.59	0.05	0.84	0.06	0
Alloy:	Total	Electricity	Direct	Kerosene	Lime	Extractant	Caustic soda	Steam	Oxygen	Sulfuric acid	Water	
AP	79.03	0.21	0	8.26	0.03	5.36	20.61	4.79	2.44	37.26	0.05	
ADP	61.27	0.27	0	0.64	0.01	5.82	36.73	0.37	0.84	16.55	0.04	
GWP	47.66	0.48	0	4.04	0.03	7.38	21.74	8.88	2.76	2.28	0.06	
EP freshw.	75.27	0.51	0	1.43	0.07	6.36	45.87	3.78	12.13	4.93	0.19	
EP marine	52.96	0.37	0	7.01	0.06	6.48	28.14	4.63	2.86	3.35	0.07	
EP terrestr.	56.96	0.41	0	8.06	0.06	7.22	29.48	5.20	2.64	3.81	0.07	
HTP canc.	69.27	0.47	0.00	4.02	0.06	18.52	30.77	4.33	1.98	8.56	0.56	
HTP non-c.	69.47	0.43	0.00	4.46	0.03	5.96	42.42	2.82	2.68	10.33	0.33	
ODP	90.85	0.21	0	27.87	0.01	2.66	53.24	5.14	0.56	1.15	0.02	
POCP	70.57	0.40	0	11.88	0.06	11.35	28.36	6.08	2.61	9.76	0.08	

Dust:	Total	Electricity	Soda	Direct	Steam	Water						
AP	6.66	0.02	6.53	0	0.11	0.01						
ADP	17.20	0.02	17.17	0	0.01	0.00						
GWP	8.11	0.04	7.87	0	0.20	0.01						
EP freshw.	10.53	0.04	10.38	0	0.08	0.02						
EP marine	27.26	0.03	27.12	0	0.10	0.01						
EP terrestr.	10.83	0.03	10.68	0	0.12	0.01						
HTP canc.	15.57	0.04	15.37	0	0.10	0.07						
HTP non-c.	12.26	0.03	12.13	0	0.06	0.04						
ODP	1.80	0.02	1.67	0	0.11	0.00						
POCP	8.50	0.03	8.32	0	0.13	0.01						
Credits:	Total	Copper	Aluminum	CoSO₄	NiSO₄	Li₂CO₃						
AP	-510.67	-163.29	-13.14	-62.42	-231.59	-40.32						
ADP	-5541.17	-2857.38	-2.35	-902.61	-1682.67	-96.16						
GWP	-142.73	-11.87	-10.91	-34.84	-58.56	-26.55						
EP freshw.	-618.49	-347.19	-21.29	-61.18	-118.44	-70.39						
EP marine	-351.94	-51.98	-11.90	-57.81	-112.23	-118.02						
EP terrestr.	-272.30	-77.03	-12.57	-41.38	-85.50	-55.81						
HTP canc.	-6044.37	-400.46	-60.74	-1948.78	-3592.25	-42.14						
HTP non-c.	-2077.73	-1195.73	-36.62	-279.13	-495.58	-70.67						
ODP	-69.23	-2.60	-3.30	-20.26	-31.54	-11.53						
POCP	-307.23	-76.69	-14.98	-48.88	-119.07	-47.61						

pt-LFP

Pre-treat:	Total	Electricity	Natural gas	Lime	Diesel	Direct	Nitrogen	Water				
AP	14.82	0.52	1.52	0.16	11.67	0	0.94	0.01				
ADP	1.65	0.55	0.33	0.06	0.35	0	0.36	0.00				
GWP	12.93	0.40	3.31	0.06	1.68	7.12	0.36	0.00				
EP freshw.	3.10	0.55	0.22	0.16	0.12	0	2.03	0.02				
EP marine	20.69	0.46	1.52	0.16	17.96	0	0.58	0.01				

EP terrestre.	24.49	0.53	1.79	0.17	21.44	0	0.55	0.01				
HTP canc.	0.34	0.08	0.12	0.02	0.06	0	0.05	0.01				
HTP non-c.	5.30	0.68	0.56	0.11	3.24	0	0.67	0.04				
ODP	20.85	0.94	11.30	0.09	8.10	0	0.41	0.01				
POCP	17.45	0.39	1.62	0.12	14.91	0	0.40	0.01				
Pyro:	Total	Electricity	Lime	Coke	Silica	Direct	Calcium chloride	Air	Natural gas	Water	BF slag	Limestone
AP	57.00	1.08	0.08	23.66	7.37	0	21.47	3.34	0.04	0.10	1.57	1.63
ADP	50.63	1.14	0.03	1.58	1.26	0	41.38	5.24	0.01	0.05	0.57	0.28
GWP	76.17	0.81	0.03	7.09	1.92	62.26	2.90	1.16	0.08	0.04	0.58	0.25
EP freshw.	77.35	1.13	0.08	57.78	2.09	0	9.49	6.78	0.01	0.15	0.37	0.16
EP marine	33.77	0.96	0.08	16.83	6.37	0	7.66	1.87	0.04	0.06	1.89	1.94
EP terrestre.	49.73	1.09	0.08	17.11	7.29	0	22.35	1.81	0.05	0.07	2.21	2.81
HTP canc.	95.83	0.16	0.01	93.04	0.41	0	1.86	0.35	0.00	0.07	0.13	0.06
HTP non-c.	63.05	1.40	0.05	31.94	3.50	0	22.38	3.78	0.01	0.37	1.29	0.64
ODP	32.29	1.93	0.04	21.10	3.64	0	4.29	1.29	0.29	0.05	2.56	1.00
POCP	66.06	0.79	0.06	53.28	5.53	0	5.06	1.34	0.04	0.06	1.69	1.70
Alloy:	Total	Electricity	Direct	Kerosene	Lime	Extractant	Caustic soda	Steam	Oxygen	Sulfuric acid	Water	
AP	7.55	0.04	0	0.71	0.00	0.71	6.09	0	0.18	0.00	0.00	
ADP	9.78	0.04	0	0.05	0.00	0.65	9.04	0	0.05	0.00	0.00	
GWP	2.64	0.03	0	0.12	0.00	0.33	2.16	0	0.07	0.00	0.00	
EP freshw.	6.43	0.04	0	0.05	0.00	0.37	5.97	0	0.40	0.00	0.00	
EP marine	5.07	0.03	0	0.31	0.00	0.44	4.29	0	0.11	0.00	0.00	
EP terrestre.	5.55	0.04	0	0.37	0.00	0.51	4.63	0	0.11	0.00	0.00	
HTP canc.	0.82	0.01	0.00	0.02	0.00	0.17	0.62	0	0.01	0.00	0.00	
HTP non-c.	8.91	0.05	0.00	0.25	0.00	0.51	8.10	0	0.13	0.00	0.01	
ODP	34.23	0.07	0	4.45	0.00	0.65	29.06	0	0.08	0.00	0.00	
POCP	4.30	0.03	0	0.40	0.00	0.59	3.28	0	0.08	0.00	0.00	
Dust:	Total	Electricity	Soda	Direct	Steam	Water						
AP	17.29	0.06	16.93	0.00	0.28	0.02						

ADP	37.12	0.07	37.02	0.00	0.02	0.01							
GWP	7.09	0.05	6.86	0.00	0.17	0.01							
EP freshw.	12.05	0.07	11.85	0.00	0.10	0.03							
EP marine	36.42	0.06	36.21	0.00	0.14	0.01							
EP terrestre.	14.92	0.06	14.69	0.00	0.16	0.01							
HTP canc.	2.76	0.01	2.72	0.00	0.02	0.01							
HTP non-c.	20.55	0.08	20.30	0.00	0.10	0.07							
ODP	8.66	0.11	7.99	0.00	0.55	0.01							
POCP	8.64	0.05	8.44	0.00	0.14	0.01							
Credits:	Total	Copper	Aluminum	CoSO₄	NiSO₄	Li₂CO₃							
AP	-960.13	-796.27	-59.58	0	0	-104.28							
ADP	-11809.23	-11592.99	-8.86	0	0	-207.37							
GWP	-59.33	-19.50	-16.66	0	0	-23.17							
EP freshw.	-868.64	-745.76	-42.52	0	0	-80.36							
EP marine	-315.96	-130.58	-27.81	0	0	-157.58							
EP terrestre.	-306.45	-199.40	-30.26	0	0	-76.79							
HTP canc.	-159.38	-133.15	-18.78	0	0	-7.45							
HTP non-c.	-3991.30	-3765.74	-107.27	0	0	-118.29							
ODP	-106.22	-23.43	-27.63	0	0	-55.15							
POCP	-221.37	-146.44	-26.60	0	0	-48.33							

S3.4. Sensitivity analysis

Unlike the rest of the assessment, the sensitivity analyses were represented as a black box model consisting of the whole process (pre-treatment, reducing smelting, alloy refining, and lithium dust refining) and the avoided burden credits. The results are provided in **Table S13**.

Table S13. Results of the sensitivity analysis: impact assessment and the change in impacts vs. baseline *pt* black mass.

	<i>L-III</i>			<i>L-8II</i>			<i>L-LFP</i>		
	Process	Credits	vs. <i>pt</i> -111	Process	Credits	vs. <i>pt</i> -811	Process	Credits	vs. <i>pt</i> -LFP
AP (mol H ⁺ eq)	22.92	-140.00	+4.09%	26.39	-129.12	+4.83%	8.04	-61.20	+26.07%
GWP (kg CO ₂ eq)	3570	-8520	-5.93%	3860	-5980	-7.13%	3240	-1860	+3.57%
EP freshwater (kg P eq)	1.06	-6.83	+28.79%	1.18	-5.79	+26.41%	0.82	-4.66	+51.99%
EP marine (kg N eq)	3.78	-17.14	+7.20%	4.08	-13.33	+8.19%	2.20	-5.85	+18.87%
EP terrestrial (mol N eq)	35.32	-121.72	+7.30%	38.56	-97.49	+8.30%	20.35	-52.06	+19.68%
HTP cancer (CTUh)	5.96E-6	-1.71E-4	+254.90%	6.24E-6	-1.14E-4	+235.12%	1.19E-5	-1.10E-5	+72.61%
HTP non-cancer (CTUh)	4.56E-5	-1.18E-3	+10.30%	5.05E-5	-9.55E-4	+10.33%	2.36E-5	-7.17E-4	+31.33%
ODP (kg CFC-11 eq)	9.16E-4	-1.09E-3	+5.42%	1.08E-3	-7.19E-4	+5.38%	2.45E-4	-1.50E-4	+73.76%
POCP (kg NMVOC eq)	11.16	37.28	+27.34%	12.47	-30.53	+26.18%	9.39	-14.15	+46.75%
ADP (kg Sb eq)	3.72E-2	-2.47	+1.42%	3.54E-2	-1.94	+1.62%	1.16E-2	-1.25	+9.30%

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