Life Cycle Modelling of Extraction and Processing of Battery Minerals – A Parametric Approach

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Table S1. Assumptions and range of values for parameters used in model.

Value Chain	Process Stage	Levers (Parameters)	Parameter Description	Range	References	Number of distinct LCA Simulations
		Mine Type	The type of mine determines the mining operations carried out. As underground mining presents distinct properties from open-cast (also called open pit) mining, the life cycle inventory, especially the energy use, is also different for these mine types. We include this as a parameter in copper mining to test its effect on the GWP.	[Underground, Open-Cast]	[1]	
Copper	Mining and concentration	• Mine depth	For underground mines, the depth of the mine determines the efforts and consequently energy required to sustain mining operations. We adopt mine depth as a parameter as this allows us to calculate the efforts (energy use) as a function of the mine depth. Consequently, the GWP will vary as a function of the depth. We use 450m as the maximum for our simulations.	[0 - 450m]	[1]	300
		Ore grade	Ore grade is a typical characteristic of copper mining operations, and this determines the efforts needed to extract the mineral from the ground. More rock material is required to be mine at low copper ore grades than high at ore grades. This variation in the ore grade affects the mining energy and molar concentration of reactants to process the ore. Ore grades determine the energy and material consumption at mining sites. We, therefore, adopt this as a parameter to	[1 - 5%] copper	[1][2]	

				investigate its effect on the			
		•	Recovery Efficiency	GWP. The recovery efficiency applied for the concentration phase measures how concentrated ore is recovered without waste (material waste). At lower concentrate recovery efficiency, more material and energy is needed to produce a unit of the desired material that is being wasted due to the loss in recovery efficiency. This idea prompts us to adopt the recovery efficiency of the	[80 - 96%]	[3]	
		•	Carbon Intensity of Electricity Mix	copper concentration phase into a parameter. The energy intensity of the mix measures the GHG emissions of the electricity mix used in the copper concentration phase.	[0.2 - 1.1] kgCO:e/kWh	[4],[5]	
	Smelting and	•	Recovery Efficiency	Converting copper concentrate into copper matte through smelting also considers the matte's recovery efficiency, which measures how effectively the matte is recovered after production. We include this recovery for the smelting process (conversion into matte) and refining into pure metal as parameters.	[80-96%]	[6]	
	Refining	•	Smelting Technology	In copper smelting, various smelting technologies have different energy requirements and material consumption. According to the technologies, we adopt smelting technology as a parameter in our model due to energy and process efficiency variations.	Flash, Isasmelt, Mitsubishi, KH- Outokumpu Flash, KH-Hot Calcine Reverb	[7]	150
		•	Carbon Intensity of electricity mix	Same as in copper mining and concentration	[0.2 - 1.1] kgCO:e/kWh	[4],[5]	
Aluminum	Bauxite and Alumina	•	Bauxite ore grad	The alumina content in bauxite ore, also called bauxite ore grade or resource quality, determines how much effort (energy and material) is consumed to produce a unit of alumina from the bauxite. At low bauxite resource quality, more bauxite is needed to be mined to produce a unit of alumina, consequently increasing energy and material consumption.	[31 - 52%] Alumina content	[8]	289
		•	Overburden to bauxite ratio	Overburden refers to the topsoil layer which must be removed to extract the bauxite resource. The	0.02-6	[8]	

			thickness of the overburden			
			layer determines the amount of material to be dug up			
			before accessing the bauxite			
			resource. This overburden			
			layer can range from 0-20m in			
			some mines. The ratio of the thickness of the overburden			
			layer to the thickness of			
			bauxite layer is used as a			
			parameter to determine the			
			amount of material to be extracted before accessing the			
			bauxite resource which			
			directly determines the			
			energy requirements of the			
	•	Recovery	process. Recovery efficiency in the	[70-95%]	[9]	
		Efficiency	bauxite and alumina stages	[70-95/6]	[2]	
		Linciency	refers to the effectiveness of			
			recovering the bauxite mined			
			for the mining stage and			
			recovering the alumina produced in the Bayer			
			process. This recovery			
			efficiency determines the			
			material and energy use. Like			
			recovery efficiency in the copper concentration process			
	•	Carbon	The energy intensity of the	[0.2 - 1.4]	[10],[5]	
		intensity of	mix measures the GHG	kgCO2e/kWh		
		electricity mix	emissions of the electricity			
			mix used in the bauxite			
			mining and Bayer process. Some mining operations			
			used direct electricity from			
			grid while others used fossil			
			fuels to produce electricity on			
			site for mining operations. Similarly, for the Bayer			
			process, grid electricity can be			
			used, or direct electricity			
			produced on the process			
	•	Technology type	plant. For the electrolysis stage, the	[Prebake,	[11]	
			prebake and the Søderberg	Søderberg]	[]	
			technologies have been			
			commonly used. Within the			
			prebake technology, the point feeder prebake (PFPB), the			
			centre work prebake			
			(CWPB), and the side work			
			prebake (SWPB) are also			
Electrolysis			available. Similarly, within the Søderberg technology, the			
and ingot			horizontal stud Søderberg			289
casting			(HSS) and the vertical stud			
			Søderberg (VSS) exists. We			
			adopt the average values for the prebake and the			
			Søderberg technologies as			
			representative technologies of			
		D	the sub-variants.	[00,000/3	[7]	
	•	Recovery efficiency	Recovery efficiency parameter in the Hall-Heroult	[80-98%]	[6]	
		emdericy	process refers how to the			
			effectiveness in fully			
					·	

				obtaining the primary liquid produced.			
		•	Carbon intensity of the electricity mix	The intensity of the carbon intensity is a very important parameter for this as there is high energy consumption in this stage, so the source of electricity is simulated as a parameter	[0.2 - 1.4] kgCO:e/kWh	[5]	
		•	Energy efficiency improvements	Due to the high electricity consumption in the aluminum smelting process, the effects of increasing energy efficiency are considered as a parameter to capture the efforts of smelting industries increasing energy efficiency.	[2-10%]	[12]	
		•	Mine Type	Mine type for this process is like the copper mining process	[Underground, Open-Cast]	[13,14]	
	Mining and concentration	•	Ore grade	Ore grades follow a similar explanation like for the copper mining process. However, nickel ores have lower grades than copper ores. In most mining operations, the ores extracted contain various proportions of copper, nickel, and cobalt metals.	[1,5 – 3,5%] nickel content	[15]	280
		•	Recovery Efficiency	Recovery efficiency follows the same thinking as explained in the copper mining and concentration process	[80 -90%]	[6]	
Nickel		•	Carbon intensity of electricity mix	The consideration of this parameter follows similar explanation as other carbon intensities of electricity mix described above	[0.2 - 1.1] kgCO:e/kWh	[16], [5]	
	Smelting and Refining	•	Recovery Efficiency	This parameter follows similar explanation as the recovery efficiency for copper smelting and aluminum electrolysis previously explained	[85 - 96%]	[6]	160
		•	Carbon Intensity of electricity mix	This parameter is the same as the one for copper smelting previously described.	[0.2 - 1.1] kgCO:e/kWh	[16],[5]	
		•	Energy Efficiency improvements	Energy efficiency in the smelting process here follows a similar explanation as energy efficiency in the aluminum smelting process previously explained.	[2-14%]	[17]	
Manganese	Mining and Concentration	٠	Ore grade	The explanation of manganese ore grade is as those of copper, nickel and bauxite ore grades previously explained. However, manganese has very high ore grades compared to copper and nickel.	[10 -50%]	[18,19]	119
		•	Recovery Efficiency	This follows similar explanation as for copper and nickel mining and	[80 - 96%]	[20]	

			concentration previously explained.			
		Carbon efficiency of electricity mix	Follows similar explanations as the for the value chains explained above.	[0.2 - 1.4] kgCO2e/kWh	[21][5]	
	Smelting and Refining	Recovery Efficiency	Follows similar explanation for the smelting and refining processes for the value chains previously explained.	[80 -96%]	[18,20]	145
		Carbon Intensity of electricity mix	Similar description as for the other value chains previously described.	[0.2 - 1.4] kgCO:e/kWh	[21][5]	
	Natural graphite	Ore grade	Natural graphite can exist in amorphous or flake forms. Amorphous graphite has higher ore grades by carbon content measured in 50 to 90% C content. However, amorphous carbon is not suitable for battery applications and is primarily used in refractories. The ore grades used in this study represent those of flake graphite which are practical for battery anode production. The flake graphite ore grade also determines the amount of energy and other inventories used in the mining and the beneficiation, as previously explained for the value chains above.	[7 -20%]	[22]	119
Graphite		Recovery Efficiency for mining and beneficiation Carbon intensity of	Recovery efficiency for the graphite value chain follow similar explanation as for those of other value chains already described above. Carbon intensity of electricity mix is used as parameter as explained in the previous	[80 - 96%] [0.2 - 1.4] kgCO:e/kWh	[0.2 - 1.4]	
		electricity mix	value chains	FA 1	[04]	
		Technology choice	The Acheson and the Castner furnaces have different energy requirements and configurations which leads to various impacts and are therefore modeled as parameter.	[Acheson, Castner]	[24]	
	Synthetic graphite	Recovery efficiency for synthetic graphite production	The recovery efficiency of synthetic graphite determines the inputs of pitch and coke and energy used for the baking and graphitization process which changes the overall impacts as already explained in the value chains previously described.	[80 - 96%]	[23][25]	59
		Carbon intensity of electricity mix	Carbon intensity of electricity mix is used as parameter as explained in the previous value chains	[0.2 - 1.4] kgCO:e/kWh	[0.2 - 1.4]	
Lithium Carbonate	Spodumene Route	Ore grade	Spodumene ore grades affect the amount of energy used in mining as well as the quantity of reactants used in the concentration process as	[0.58 – 2%]	[26]	39

	Recovery Efficiency for spodumene mining and lithium carbonate production	previously explained for the value chains above This parameter characterizes the material recovery efficiency for both the mining and the concentration process.	[70 -95%]	[27]	
	Carbon intensity of energy mix	Carbon intensity of electricity mix is used as parameter as explained in the previous value chains.	[0.2 - 1.0] kgCOæ/kWh	[21][5]	
Brine Route	Brine Quality	This parameter determines the conditions for brine evaporation. High quality means the brine is extracted using solar evaporation only, while for low quality, solar evaporation and additional heating provided by natural gas is used	[Low Quality, High Quality]	[28]	20
	Recovery Efficiency for brine extraction and lithium carbonate production	Like other recovery efficiencies for other value chains previously described.	[70 -95%]	[27]	

For consecutive unit processes in the value chain, the recovery efficiency η is used in the foreground defined as:

$$\textit{Quantity of material}_{process \ i} = \frac{\textit{element content in process}_i}{\textit{element content in process}_{i-1}} * \eta$$

Recovery efficiency signifies the degree to which the material produced is effectively recovered without losses (a measure of production or conversion losses). This means that at an η of 100%, all the element contained in process i-1 is converted without any losses in process i. This applies to all the processes in the value chains described below.

In addition, for all value chains investigated, the carbon intensity of the mix for different geographic regions are evaluated from ecoinvent v3.2 [5] using the LCA activity browser tool [29].

1. Copper

1.1 Copper Mining and Concentration

For the energy used in copper mining and beneficiation, we use ore-grade energy equations from references [1,30–32] as shown in Table S2.

The copper ore grade represents the copper element content in a quantity of material extracted expressed as a %.

Table S2: Energy used in copper mining and concentration

	Energy Used	Explanation	Author	
	$15.697 * G^{-0,573}$	G is ore grade	Northey et al.(2013)	
Tatal Minima and	$15.63 * G^{-0,529}$		Kuipers et al. (2018)	
Total Mining and Concentration	$23.81 * G^{-0,529}$		Valero and Valero (2014)	
Energy	В	D is mine depth in metres		
Energy	$\alpha + \gamma \cdot D + \frac{\beta}{G}$	G is ore grade		
		α, γ, β are fitting parameters	Koppelaar and Koppelaar	
Diesel	$1.564 - 0.00073 * D + \frac{0.0064}{G}$		(2016)	
	$1.569 + 0.00066 * D + \frac{0.0067}{G}$	D is depth in meters and G is ore		
Electricity	G	grade in %		

Other inventories for the mining and concentration phase relate to the ore grade following regressed relationships from ecoinvent v3.2. These relationships are of the form A. $G^{-\alpha}$; where A and α are fitting coefficients and G is the ore grade.

1.2 Copper Smelting

Data for energy used in copper smelting is taken from Coursol et al. [7] as illustrated in Table S3.

Table S3: Energy requirements for Copper Smelting

Smelting Route	Electric Energy(kWh/kg)	Fossil Fuel(MJ/kg)
Flash	0,979	1,518
Isasmelt	0,729	4,175
KHCalcineR	0,196	15,9
KHMitsubishi	0,623	9,3
KHNoranda	0,817	5,22
KHOutokumpuF	0,675	6,76
Mitsubishi	0,898	2,498
Noranda_ElTeniete	1,065	2,657

1.3 Copper Electricity Mix Intensity

Electricity mix for the 9 regions are used for the background process parameters for copper simulation as shown in Table S4.

Table S4: Electricity mix for Copper Value Chain

	RSA	RAF	RND	RNA	Canada	European Average	China	Australia	Russia
Hydropower electricity	35,2 %	30,7 %	34,6 %						
Natural gas electricity	25,6 %	0,0 %	2,0 %	Ecoinvent V3.2 background processes					
Coal electricity	20,3 %	62,3 %	5,0 %						
Nuclear electricity	1,3 %	3,7 %	40,5 %						
oil electricity	4,3 %	1,7 %	0,3 %		ECC	omvent vs.z backgro	una proces	5565	
Wind power	4,7 %	1,3 %	10,3 %						
Biofuels/waste	6,1 %	0,1 %	7,2 %						
Solar PV	2,5 %	0,2 %	0,3 %						

RSA: South America (Argentina, Bolivia, Chile, Brazil, Colombia, Mexico, Peru)

RAF: Africa (Zambia, Congo, South Africa)

RND: Nordics (Sweden, Finland)

RNA: North America (excluding Canada)

To ensure that we allocate an electricity mix that matches the production percentages within a region, the percentages of electricity mix for the regions RSA, RAF, RND, and RNA in Table S4 represent the weighted average of the total quantity of copper produced and the electricity mix for each country within the region. This mix is calculated as follows:

$$\begin{aligned} &Regional \ electricity \ of \ mix \ for \ energy \ technology_i \\ &= \frac{\sum_{1}^{n} \left(\frac{copper \ production_{j}}{\sum_{1}^{n} copper \ production}\right) * country \ generation \ of \ energy \ technology_i}{Total \ regional \ generation} \end{aligned}$$

Where n is the number of production countries and i is the generation technology.

2. Aluminum value Chain

2.1 Bauxite Mining

The total quantity of bauxite mined per unit alumina produced is taken from Ter Weer [33] and as expressed as:

bauxite mined =
$$\frac{1}{\eta_{baux} * B} * \frac{1}{\alpha * \eta_{alum}} * (1 + e)$$

 η_{baux} : Mining recovery (dry basis).

B: Beneficiation(also referred to as "ore concentration") recovery, % (dry basis). For a project not applying beneficiation, B is considered to be 100%.

α: Percentage available alumina, otherwise called bauxite quality or bauxite ore grade, % (dry basis).

 η_{alum} : Alumina recovery efficiency %.

e: Overburden/bauxite ratio, representing the total ground to be dug before reaching a bauxite resource.

2.2 Alumina Processing

For alumina processing by the Bayer process, we assume that the bauxite resource quality will also affect the quantity of materials and energy used to produced alumina. As such, lower bauxite quality will require more caustic soda, material inventory, and energy. However, due to the complexity in modelling this relationship, we adopt a mathematical approach that permits us to scale the materials and energy as a function of the bauxite quality. We begin with a global bauxite resource average of 41%, which translates into approximately 2.5 kg of bauxite per kg of alumina produced and corresponds to the base inventory adopted. We define a factor k (allows for the proportionate scaling of the base inventory), which is the ratio of the quantity of bauxite used in the Bayer process at a given ore grade (α) to the bauxite used at 41% alumina content.

$$k = \frac{bauxite\ quantity\ at\ \alpha\ grade}{bauxite\ quantity\ at\ 41\%\ ore\ grade}$$

$$k = \frac{\frac{1}{\eta_{baux} * B} * \frac{1}{\alpha * \eta_{alum}} * (1 + e)}{2.5}$$

For simplicity, we assume there is no beneficiation (B=100%). Therefore, k can be expressed as follows

$$k = \frac{\frac{1}{\eta_{baux}} * \frac{1}{\alpha * \eta_{alum}} * (1 + e)}{2.5}$$

2.3 Aluminum Smelting

For aluminum smelting, we use the energy for prebake and Søderberg technologies taken for International Aluminum Institute [11,34], as shown in Figure S1. In addition, we include the energy improvement efficiencies, which captures reduction in energy used for the electrolysis phase.

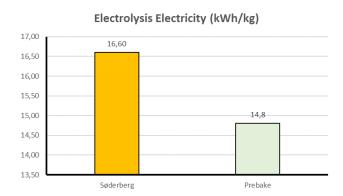


Figure S1: Electricity use for aluminum electrolysis

If γ is the energy improvement efficiency (%), the new energy value becomes:

$$E_{paramaterized} = (1 - \gamma)E_{base\ inventory}$$

2.4 Aluminum Electricity Mix

The set of values of electricity mix for aluminum production is from ecoinvent v3.2, however, we add a designed mix specifically for the Nordic region as shown in Table S5.

Table S5: Electricity mix for aluminum Value Chain

	RND	EU 27 &EFTA	IAI 1	IAI 2	IAI 3	IAI 4 & 5	RUS/RER	CNA	OCE	GCC	CAN
Hydropower electricity	90,2 %										
Natural gas electricity	1,6 %										
Coal electricity	0,2 %										
Nuclear electricity	3,9 %		Ecoinvent v3.2 background processes								
oil electricity	0,0 %										
Wind power	3,4 %										
Biofuels/waste	0,6 %										
Solar PV	0,0 %										

RND: Nordic Region

Description of the regional electricity mix classification (for the ecoinvent v3.2 background processes) in Table S5 can be found on the https://geography.ecoinvent.org/

3. Manganese Value Chain

3.1 Manganese Mining and Concentration

The energy for mining and concentrating manganese ore is taken from reference [19] given by the formula:

$$E = 143.7G^{-1}$$

Where G is the ore grade

The energy E is split into diesel and electricity by using ratios from ecoinvent v3.2, which yields 25%

for electricity and 75% for diesel.

To further parameterize the mining and ore concentration phase, we assume that all the materials used for this process stage will relate to the ore grade following an inverse relationship of the form

$$material\ inventory = A.G^{-1}$$

Where G is the ore grade and A is a fitting coefficient.

Based on ecoinvent data of G=35.7%, we proceed to calculate the value of A for each material in the inventory list. This permits us to deduce a generic following relating ore grade and material inventory for the mining and concentration stage of the manganese value chain.

3.2 Production of electrolytic manganese metal (EMM)

Apart from a recovery efficiency applied to this phase, there is no change in the inventories. Inventories are taken from econovent v3.2.

3.3 Electricity mix for Manganese

The range of the mix for manganese value chain is taken to represent that of major producing countries as shown in Table S6.

Table S6: Electricity mix for Manganese Value Chain

Australia	Brazil	Canada	China	India	France	Japan	Norway
Ecoinvent V3.2 electricity mix (medium voltage)							

4. Nickel Value Chain

4.1 Nickel Mining and Concentration

The energy used to mine and concentrate nickel ore is expressed as a function of the ore grade and mine type according relationship calibrated with data from references [6,35] as shown in Table S7. Similarly, the quantity of explosives use to mine a ton of ore is taken from reference [35] which calculates this at 1.1kg of explosive per kg of ore mined. We transform this into a relationship to include ore grade as shown in Table S7:

Table S7: Energy and explosive requirements for Nickel Mining

	Underground Mine	Open Cast
Diesel (MJ/kg Ni)	$6.6*G^{-1}$	$14.1 * G^{-1}$
Electricity (kWh/kg Ni)	$9.6 * G^{-1}$	$7.2 * G^{-1}$
Explosives (kg)	0.11 *	G^{-1}

4.2 Nickel Matte and Nickel Refining

All the inventories for nickel matte are taken from reference [13] except the energy used in smelting which is the average of the INCO and Fortaleza smelters taken from reference [35]. Inventories for

nickel refining are taken from [13] except the energy use which is taken from [6].

We also include the effect of efficiency improvements (γ in %) in energy used as :

$$E_{parameterize} = (1 - \gamma)E_{base\ inventory}$$

4.3 Electricity mix for Nickel

The range of the electricity mix for nickel value chain is taken to represent that of major producing countries as shown in Table S8.

Table S8: Electricity mix for Nickel Value Chain

Australia	Brazil	Canada	China	Europe	Finland	Russia	South Africa	China	Europe	Japan
Ecoinvent V3.2 electricity mix (medium voltage)										

5. Graphite

5.1 Natural Graphite

For natural graphite, the energy used for mining and beneficiation is taken from [36]. We adopt the generic energy-ore equation of the form $E = A.x^{-0.5}$, which is taken from [32]. Using an ore grade of 6.24% C content taken from same reference, we calibrate the fitting parameters A for diesel, electricity, and natural gas. The energy requirements are displayed in Table S9.

Table S9: Energy requirements for natural graphite

Diesel (MJ/kg)	$26.1 * G^{-0.5}$
Natural gas (MJ/kg)	$6.118 * G^{-0.5}$
Electricity (kWh/kg)	$2.67 * G^{-0.5}$

5.2 Synthetic Graphite

Synthetic graphite is modeled with inventory from reference [25], we distinctly model the graphitization energy used for Castner and Acheson furnaces based on lower and upper limit data from [24].

Table S10: Energy requirements for Castner and Acheson furnaces

	Lower Limit (kWh/kg)	Upper Limit (kWh/kg)
Castner Furnace	2	3
Acheson Furnace	3	4

The upper limits of the energy used in graphitization may increase than the stated values in Table S10 as suggested by reference [37], but due to lack of high resolution data, we use these numbers from [24,25] as a good approximation for our parametric modelling.

For synthetic graphite, we include the conversion efficiency η from reference [25], which measures the efficiency in converting petroleum coke and coal tar pitch to synthesized graphite as.

$$\eta = \frac{quantity \ of \ graphite \ synthesized}{coal \ tar \ input + \ petrol \ coke \ input}$$

5.3 Electricity mix for Graphite

The carbon intensity of the mix for graphite electricity regions are shown in Table S11.

Table S11: Electricity mix for graphite value chain

Canada	China	India	Russia	Norway	Ukraine	Brazil	
Ecoinvent V3.2 electricity mix (medium voltage)							

6. Lithium Carbonate

6.1 Lithium carbonate from spodumene

The relationship between ore grade (G) and energy used (E) for mining and concentration of spodumene is taken from [32], given by

$$E = 3.58. G^{-0.5}$$

From the percentage of diesel and electricity used in mining and concentration from [28], we split the energy (E) used for mining and concentration of spodumene which yields 35% electricity and 65% diesel.

We further base our material inventory assumptions for mining and concentration of spodumene on those from reference [28], which uses an inverse proportion to scale material inventory to the ore grades. From reference [28], when the ore grade (Lithium content) increased from 0.58% to 1.86% (a factor of 3.21), the inventory reduced by approximately the same factor. We use the inventory for an ore grade of 0.58% as the base inventory and scale other material inventories to this base inventory.

The scaling factor k for each inventory element for mining and concentration is thus calculated by:

$$k = \frac{0.58\%}{Ore\;grade\;(G\;in\;\%)}$$

The base inventory of carbonation of spodumene to lithium carbonate from reference [28] is only modified by including a recovery efficiency in the carbonation process.

6.2 Lithium carbonate from Brines

The base inventory for "high grade" brine is taken from [28]. For "low grade" brine, we use the inventory from [38] which includes the extra energy from natural gas to heat up the brines. Recovery efficiency is also included in the brine extraction and carbonation process. The electricity mix for the different countries investigated are shown in Table S12.

Table S12: Electricity mix for Lithium Carbonate

	Sp	odumer	Brine					
Australia China		Brazil	Portugal	Finland	Chile	Bolivia	Argentina	
Ecoinvent V3.2 electricity mix (medium voltage)								

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