Life Cycle Environmental Assessment of Lithium-Ion and Nickel Metal Hydride Batteries for Plug-in Hybrid and Battery Electric Vehicles. Supporting Information

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1 System description and general inventory considerations

Figure S1a presents our battery system, defined by the delivery of 50 MJ of electrical energy to the power-train. The production chains of the the different electrode pastes batteries were inventoried as presented in Figure S1b-f. Unless otherwise specified, the different process descriptions assume average European conditions. This choice is motivated by a greater data availability. Except for the final delivery of the battery, the transportation requirements were all based on standard transportation distances formaterials consumed in Europe, as reported in Ecoinvent (1). The infrastructure requirements of this inventory were all assessed with proxies from Ecoinvent.

Figure S1. General flow diagram of the FU and battery system (a), along with detailed flow diagrams of the different electrode pastes (b-f). The different electrode pastes are highlighted in gray. *Abbreviations:* BMS refers to “battery management system”, CMC to carboxymethyl cellulose, NMP to N-methylpyrrolidinone, and PTFE to polytetrafluoroethylene.

2 Modeling battery composition

The energy density of a cell is function of its mass share of electrochemically active material. However, for fast charge and discharge currents (high power), the layer of the electrode material on the current collectors should be as thin as possible. Greater power density is thus achieved by batteries with smaller proportions of chemically active material and larger proportions of “supporting components”, as illustrated by the Ragone plot (2, 3). The share of the battery mass embodied as electrode materials, electrode substrates, separators, and containers can vary by 3-4 folds between a high-power and a high-energy battery (4) .

To model the three batteries of this study, we reconciled material electrochemical properties (specific capacity and voltage), battery dismantling inventories, and expected typical battery performances. Figure S2 illustrates the procedure followed to produce our three inventories (Table S1). First, a certain “packaging factor” had to be assumed (Figure S2, step a). The different scenarios put forth by Axsen et al. (5) present mass fractions of 25% or 16% for non-cell components, while Gaines and Nelson (6) report values of approximately 13%. Our model assumes 17% of the battery mass as packaging, plus 3% for the battery management system (BMS) for Li-ion batteries. This does not include any cooling system, which we consider to be beyond our system boundaries.

Figure S2. Procedure used to model batteries of the desired power and energy densities with different chemistries. First the mass of the non-cell components and of the electrolyte form was fixed (a, b). The share of the cell represented by of electrochemically active materials was chosen depending on the desired total energy density and the properties of the materials (c). The mass ratios of positive and negative electrodes was chosen so that they would have equal reversible charge capacities (d). The remainder of the cell mass was divided amongst the supporting materials (e).

Of all the components, the mass share of the electrolyte was found to be the most insensitive to differences in battery design, ranging from 18% of cell mass for high energy Li-ion batteries to 13.5% for high power ones (4). For the two Li-ion batteries, we allocated to electrolyte 15% of the cell mass,

i.e. roughly 12% of battery mass (Figure S2, step b). For NiMH, the aqueous electrolyte represents 9% of the mass, following the inventory by Schexnayder et al. (7).

The remainder of the cell masses were “designed” so as to obtain realistic high-energy performances for all three investigated chemistries. The amounts of electrode pastes were chosen so that the product of their charge capacities and their nominal voltage would yield a credible energy density for the battery (Figure S2, step c). Furthermore, the mass proportions between positive and negative electrode pastes were chosen so that both electrodes would have an identical reversible charge capacity (Figure S2, step d). In the inventories by Gaines and Cuenca (4), the mass ratios between the remaining “supporting” components was fixed, regardless of the energy/power density design. The remainder of the Li-ion battery was thus divided between cathode current collector, anode current collector, separator material and container components according to these ratios (Figure S2, step e). The same approach was used to quantify the supporting components for the NiMH batteries, with the ratios based on the inventories by Schexnayder et al. (7) and Ying et al. (8).

Figure S2 presents conceptually how our inventories were constructed so as to be representative of PHEV and BEV technologies. Practically, the state of the art electrochemical properties of the different electrode materials were reported in Table S1-I. Based on these, the inventories of Singh et al. (9), Gaines and Cuenca (4), Schexnayder et al. (7), and Ying et al. (8) were combined and retrofitted (Table S1-II) so that they should yield credible PHEV and BEV battery performances representative of industry expectations (Table S1-III). The *total lifetime specific energy capacities* of the batteries were reported in (Table S1-IV), and their calculations detailed in Section 3.

Table S1: Electrochemical characteristics, component mass breakdown and performance of three modeled traction batteries

	NiMH	Li-ion	
	AB ₅	NCM	LFP
I. Electrochemical Properties			
Cell voltage (V)	1.2 ^{a,b}	3.7 ^{c,d,e}	3.4 ^{e,f,g}
Capacity of pure active material, positive electrode (1C rate [†]) (mAh · g ⁻¹)	275 ^h	150 ^{c,i}	120 ^{j,k}
Capacity of pure active material, negative electrode (1C rate [†]) (mAh · g ⁻¹)	290 ^h	350 ^l	350 ^l
Cycle depth of discharge (DoD) (%)	80 ^d	80 ^{c,d,e}	80 ^{d,g}
Charge-discharge energy efficiency (%)	80 ^{m,v}	90 ^{n,o,p,q,v}	90 ^{n,o,p,q,v}
Cycle life expectancy (ca. 80% DoD) (cycles)	3000 ^{d,e,f}	3000 ^{e,f,r}	6000 ^{e,f,s}
II. Battery mass composition (%)			
Positive electrode paste	19.7 ^t	23.2 ^u	24.8 ^u
Negative electrode paste	12.6 ^t	9.4 ^u	8.0 ^u
Separator	3.8 ^{h,t,v}	3.3 ^u	3.3 ^u
Substrate, positive electrode	17.3 ^{h,t}	3.6 ^u	3.6 ^u
Substrate, negative electrode	11.1 ^t	8.3 ^u	8.3 ^u
Electrolyte	9.0 ^t	12.0 ^u	12.0 ^u
Cell container, tab and terminals	9.5 ^{h,t}	20.1 ^u	20.0 ^u
Module and battery packaging	17.0 ^{h,t}	17.0 ^u	17.0 ^u
Battery management system (BMS)	-	3.0 ^t	3.0 ^t
III. Battery Performance (Calculated from I and II)			
Nominal Cell capacity (1C rate [†]) (Ah · kg _{cell} ⁻¹)	55.5	37.9 ^r	32.3
Nominal Cell energy density (1C rate [†])(Wh · kg _{cell} ⁻¹)	66.6	140 ^{r,d}	110 ^w
Total battery pack energy density (Wh · kg ⁻¹)	55.3 ^{d,e}	112 ^e	88.0
Total battery pack power density (W · kg ⁻¹)	200-400 ^{d,e}	400-800 ^{e,r}	400-800 ^e
IV. Lifetime output (Calculated from I, II, III)			
Lifetime specific energy capacity (80% DoD) (MJ · kg ⁻¹)	478	969	1520

Based on, or in approximate agreement with: ^a Hamann et al. (10), ^b Linden and Magnussen (11), ^c Ngala et al. (12), ^d Axsen et al. (5), ^e Kalhammer et al. (2), ^f Shukla and Kumar (13), ^g Chen and Whittingham (14), ^h Ying et al. (8), ⁱ Liu (15), ^j Arnold et al. (16), ^k Le Cras et al. (17), ^l Yoshio et al. (18), ^m Ikeya et al. (19), ⁿ Karden et al. (20), ^o Shiau et al. (21), ^p Van Den Bossche et al. (22), ^q Tanaka et al. (23), ^r Kokam Co. Ltd. (24), ^s Takahashi et al. (25), ^t Schexnayder et al. (7), ^u Gaines and Cuenca (4), ^v Rydh and Sandén (26), ^w Deveney et al. (27)

3 Inventory of battery use-phase

The use-phase consists of charging and discharging the battery. Due to internal resistance, energy is lost as heat during the process. The electrical energy wasted is accounted as a requirement, and the heat is accounted as the only direct emission. Also, as the battery has a limited lifetime, a fraction of the battery assembly and final shipping is allocated to each charge-discharge functional unit.

[†] A rate of nC is defined as the current that is equivalent to the full capacity of the battery being charged or discharged in 1/n hours.

The total lifetime energy capacity (C_U^t) was equated to the energy capacity of a full charge-discharge cycle (C_U), multiplied by an 80% depth-of-discharge (DoD) and the expected cycle-life of the battery under 80% depth-of-discharge and normal use ($L_{80\%}$). The energy capacity was in turn approximated from the nominal voltage (V) and the charge capacity (C_C) of the modeled cells [eq. 1].

$$C_U^t = C_U \text{ DoD}_{80\%} L_{80\%} \approx V C_C \text{ DoD}_{80\%} L_{80\%} \quad [1]$$

This approach constitutes a “deep cycle approach”, representative of the battery use for PHEV and BEV, contrarily to shallow cycles with ca. 20% DoD for stop-and-go HEV (28). Charge capacity, DoD, and cycle-life expectancies are presented for each battery in Table S1. Since the Japanese industry is an important actor in the traction battery market (4), the transoceanic freight shipping to Europe covers the distance Honshu, Japan (29).

Table S2: Inventory of requirements and emissions for 1 MJ of battery use

Parameter	NiMH AB ₅	Li-ion NCM	Li-ion LFP
Functional unit output			
Energy stored and delivered to power-train(MJ)	1	1	1
Materials and energy			
Electricity, average UCTE (kWh)	0.20	0.10	0.10
Battery Manufacture (kg)	2.1x10 ⁻²	1.0x10 ⁻³	6.6x10 ⁻⁴
Transport			
Transoceanic freight ship (OCE) (tkm)	4.6x10 ⁻⁵	2.3x10 ⁻⁵	1.5x10 ⁻⁵
Emissions			
Waste heat to air (MJ)	0.20	0.10	0.10

4 Inventory of Li-Ion batteries production

4.1 Manufacture of Li-Ion battery and subcomponents

The positive and negative electrode pastes are typically mixed on-site at the battery assembly. A coating machine then applies a thin layer (200-250 µm for high energy cells) on both sides of the electrode substrates (metal foils) (4). The applied slurry is dried and pressed (30). The positive electrode, the separator, and the negative electrode are then sandwiched together and wound-up inside the cell container. The cells are filled with electrolyte and closed. Cells are always assembled fully discharged (all lithium ions in cathode). The cells then undergo a certain number of charge-discharge cycles and compliance tests. Finally, the cells are combined in modules and battery packs, with the necessary control circuits (4).

The material requirements were determined based on the modeled component mass ratios of Table S1. The energy requirements were discussed below in Sections 8.2 and 8.3. Water, transport, and infrastructure requirements were taken from the LCA of laptop batteries by Hirschier et al. (31).

Table S3: Li-ion battery and subcomponent production

Parameter	Amount		Sub-Inventory
	NCM	LFP	
Functional Unit Output			
Li-Ion battery, assembled (kg)			
Material Requirements			
Positive electrode paste for Li-ion battery (kg)	2.3×10^{-1}	2.5×10^{-1}	Section 4.2
Negative electrode paste for Li-ion battery (kg)	9.4×10^{-2}	8.0×10^{-2}	Section 4.3
Positive electrode substrate for Li-ion battery (kg)	3.6×10^{-2}	3.6×10^{-2}	Section 4.7
Negative electrode substrate for Li-ion battery (kg)	8.3×10^{-2}	8.3×10^{-2}	Section 4.7
Electrolyte for Li-ion battery (kg)	1.2×10^{-1}	1.2×10^{-1}	Section 4.4
Separator (kg)	3.3×10^{-2}	3.3×10^{-2}	Section 6.2
Cell container, tab and terminals (kg)	2.0×10^{-1}	2.0×10^{-1}	Section 6.1
Module and Battery Packaging (kg)	1.7×10^{-1}	1.7×10^{-1}	Section 6.3
Battery management system (BMS) (kg)	3.0×10^{-2}	2.0×10^{-2}	Section 4.8
Water, decarbonated	380	380	
Processing and Energy requirements			
Electricity, medium voltage, UCTE, at grid (MJ)	27	27	
Heat, light fuel oil, at industrial furnace 1MW	2.9	2.9	
Heat, natural gas, industrial furnace low-NO _x > 100 kW	22	22	
Transport Requirements			
Freight rail transport (tkm)	2.3×10^{-1}	2.3×10^{-1}	
Lorry >16t (tkm)	5.1×10^{-2}	5.1×10^{-2}	
Infrastructure			
Facility, precious metal refinery (SE) (unit)	1.9×10^{-8}	1.9×10^{-8}	
Emissions			
Waste heat (MJ)	52	52	

4.2 Production of positive electrode pastes for lithium ion battery (NCM or LFP)

The electrode pastes of lithium ion positive electrodes are composed of the electrochemically active material, a binder substance (ca. 5-10%) and carbon black to improve conductivity (ca. 4-10%). The inventoried active materials are lithium iron phosphate (LiFePO_4) and lithium nickel-cobalt-manganese oxide ($\text{LiNi}_{0.4}\text{Co}_{0.2}\text{Mn}_{0.4}\text{O}_2$), respectively for LFP and NCM. It is an important insight that the metal constituents of both these compounds are in their oxidized state. Throughout their production chain these elements never undergo the highly energy-intensive process of reduction to the metallic form. The use of metal salts instead of pure metals distinguishes our inventory from those of Hirsch et al. (31), Schexnayder et al. (7), and Burnham et al. (32).

The most commonly mentioned binders are poly(vinylidene fluoride) (PVDF) and polytetrafluoroethylene (PTFE), but poly(acrylonitrile-methyl methacrylate) (AMMA) is also the object of research (4, 33-36). For carbon black, little gain is observed in increasing concentrations beyond 6% (35, 36). N-methylpyrrolidinone (NMP) is the preferred solvent to give the mixture a slurry texture (4, 30, 33). The solvent is evaporated after application of the electrode material on the substrate.

In this inventory, the same mass compositions were assumed for LFP and NCM electrodes. The active material accounted for 88% of the mass, a PTFE binder for 8% and carbon black for 5%. The amount of NMP solvent was estimated at 28 g per kilo of dry electrode material, based on the Ecoinvent inventory of LiMn_2O_4 electrode (31). No infrastructure use was allocated to this process, as it would typically be performed on-site at the battery assembly plant (4). The simple mixing step is not expected to lead to any significant energy consumption, emissions, or material loss. For mass balance and simplicity, the complete evaporation of the NMP solvent (after application of the paste on the substrate) was allocated to this process instead of final assembly. The detailed inventory may be found in Table S4.

Table S4: Inventory for the production of 1 kg of positive electrode material for Li-Ion battery, either LFP or NCM.

Process	Amount	Sub-Inventory
Functional Unit Output		
Positive electrode material for Li-Ion (LFP or NCM) at plant (kg, dry)	1	
Material Requirements		
For LFP: Lithium iron phosphite [LiFePO_4] (kg)	0.87	Section 4.5
For NCM: Lithium nickel cobalt manganese hydroxide [$\text{LiNi}_{0.4}\text{Co}_{0.2}\text{Mn}_{0.4}\text{O}_2$] (kg)		Section 4.6
Carbon black, GLO (kg)	0.05	
Polytetrafluoroethylene (PTFE) (kg)	0.08	
N-methyl-2-pyrrolidone (NMP) (kg)	0.28	
Transport Requirements		
Freight rail transport (tkm)	3.8	
Lorry >16t (tkm)	0.7	
Emissions		
N-methyl-2-pyrrolidone (NMP), to air, unspecified (kg)	0.28	

GLO = global average

4.3 Production of negative electrode paste of lithium ion battery (NCM or LFP)

Most lithium ion batteries presently rely on graphite electrodes. Research into electrodes based on silicon or germanium nanomaterials, amorphous carbon, carbon nanotubes, and metal alloys is ongoing (13, 37-40). To ensure the absence of any oxygen impurity in the graphite, it is baked at 1100°C in an inert or reducing atmosphere (4). The negative electrode paste is typically composed of graphite and a PTFE or PVDF binder (ca. 5%). NMC solvent is added to the mixture, to be evaporated after the paste has been applied to the substrate (4, 30, 33).

In this inventory, the binder is assumed to be PTFE. The amount of NMP required was set equal to the requirements of the positive electrode. The energy requirement to bake the graphite was estimated from the carbon anode baking of the aluminum industry, which requires $4.8\text{--}5.2 \text{ MJ}\cdot\text{kg}^{-1}$. The NMP solvent evaporation to air was assigned to this process (instead to battery assembly, see section 4.1) for mass balance and simplicity. This process is assumed to be carried out on-site at the battery assembly plant, and consequently no facility requirement was assigned to this process (4). The inert or reducing atmosphere needed during baking was not included in this inventory due to lack of data. The inventory may be found in Table S5.

Table S5: Inventory for the production of 1 kg (dry) of negative carbonaceous electrode material for Li-Ion battery.

Process	Amount
Functional Unit Output	
Negative electrode material for Li-ion battery (kg, dry)	1
Material Requirements	
Graphite (kg)	0.95
Polytetrafluoroethylene (PTFE) (kg)	0.05
N-methyl-2-pyrrolidone (NMP) (kg)	0.28
Energy and Processing	
Heat, unspecified, in chemical plant (graphite baking) (MJ)	5.0
Transport Requirements	
Freight rail transport (tkm)	0.2
Lorry >16t (tkm)	0.1
Emissions	
Heat waste (MJ)	5.0
N-methyl-2-pyrrolidone (NMP), to air, unspecified (kg)	0.28

4.4 Production of electrolyte for Li-ion battery

The liquid electrolytes are generally composed of ca. 1 molar solutions of lithium salts in a mixture of alkylcarbonate solvents (4, 41). The solvent always includes ethylene carbonate (EC) for anode passivation (42), generally complemented with dimethyl- or diethyl- carbonates (DMC, DEC) (37). Ethylmethylcarbonate (EMC), propylene carbonate (PC), and dimethoxyethane (DME) are also mentioned (4, 42). Lithium hexafluorophosphate (LiPF_6) is now the salt of choice in the industry, in spite of its tendency to generate hydrofluoric acid (HF) upon degradation (37, 41).

The production of LiPF_6 or alkyl carbonate solvents were not modeled. Rather, generic “chemicals organic” and “chemicals inorganic” proxies were used. The simple steps of mixing the solvents and dissolving the salt were not expected to require significant energy inputs, nor lead to significant material losses or direct emissions. The infrastructure use was based on the “chemical plant, organics” from Ecoinvent . The detailed inventory may be found in Table S6.

Table S6: Inventory for the production of 1 kg of electrolyte for Li-ion battery, 1M LiPF_6 .

Process	Amount
Functional Unit Output	
Electrolyte for Li-ion Battery, 1M LiPF_6 (kg)	1
Material Requirements	
Chemicals, inorganic [proxy for LiPF_6]	0.12
Chemicals, organic [proxy for solvent]	0.88
Transport Requirements	
Freight rail transport (tkm)	0.6
Lorry >16t (tkm)	0.1
Infrastructure Requirements	
Chemical plant, organics (unit)	4.0×10^{-10}

4.5 Production of LiFePO_4

Many synthesis routes exist to produce lithium iron phosphate (LiFePO_4): solid state reaction at high temperature, co-precipitation in aqueous medium, hydrothermal synthesis, or mechanochemical activation (17). The hydrothermal path was inventoried based on the synthesis protocol of (14). An iron sulphate salt ($\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$) was reacted with phosphoric acid (H_3PO_4) and lithium hydroxide (LiOH) in water in a sealed reactor at ca. 150-200°C for 5 hours (equation 2). Stoichiometric molar ratios were used, with an iron sulphate concentration of $22 \text{ g} \cdot \text{L}^{-1}$. The LiFePO_4 precipitate was collected by suction filtration and dried at 60°C for 5h. With a similar protocol, (43) reported yields between 95-98%, depending on pH.

For this inventory, a 95% yield was assumed. Lost product and co-products were assumed to be released in the hydrosphere. Total heat requirements (q_{tot}) were modeled assuming ideal thermodynamic heating of the solvent (q_s), heat losses by the reactor during reaction (q_r), and recuperation of roughly half of the heat content of the solvents after the reaction (eq. 3).

$$q_{\text{tot}} = q_s + q_r - \frac{q_s}{2} \quad [3]$$

Heat losses during reaction were modeled as in equation 4, with constant heat flux (Φ) for a given reaction time (t_r). For the reactor, we assumed a 10 m^3 cylindrical tank, with an surface area (A) of ca. 25 m^2 , covered by an insulated mineral wool layer with a thickness (x) of 0.1 m and a thermal conductivity (λ) of $0.040 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$. We further assumed a constant external wall temperature (T_o) of 50°C and a reaction temperature (T_i) of 200°C.

$$q_r = \Phi t_r = \lambda A \frac{(T_r - T_o)}{x} t_r \quad [4]$$

The energy required for the initial heating of the solvent proved to be 2 orders of magnitude greater than the modeled reactor heat loss. The energy required to dry the product was ignored, as was the enthalpy of reaction. The inventory may be found in Table S7. It should be noted that, as by-products of the iron industry, iron sulphate is only assigned energy requirements by the Ecoinvent database. Evidently, material requirements are thus being ignored.

Table S7: Inventory for the production of 1 kg of lithium iron phosphate.

Process	Amount
Functional Unit Output	
Lithium iron phosphate (LiFePO ₄)	1
Material Requirements	
Lithium hydroxide (LiOH) (kg)	0.46
Phosphoric acid (H ₃ PO ₄) (kg)	0.65
Iron Sulphate (FeSO ₄) (kg)	1.0
Deionised water (kg)	46
Energy and Processing Requirements	
Heat, unspecified, in chemical plant (MJ)	15
Transport Requirements	
Freight rail transport (tkm)	1.3
Lorry >16t (tkm)	0.21
Infrastructure Requirements	
Chemical plant, organics (unit)	4.0x10 ⁻¹⁰
Emissions	
Lithium ion, to water, unspecified	0.10
Iron ion, to water, unspecified	1.9x10 ⁻²
Phosphate ions, to water, unspecified	3.2x10 ⁻²
Waste heat (MJ)	1.5

4.6 Production of LiNi_{0.4}Co_{0.2}Mn_{0.4}O₂

The inventory of lithium nickel cobalt manganese oxide (LiNi_{0.4}Co_{0.2}Mn_{0.4}O₂) production from lithium hydroxide (LiOH) and nickel cobalt manganese hydroxide (Ni_{0.4}Co_{0.2}Mn_{0.4}(OH)₂) was based on protocol descriptions by Liu (15) and Ngala et al. (12). The two hydroxide salts were jointly ground and pelleted, and then precalcinated at 450°C for 12h. The material was then reground, repelletized, and then heated for 8h at ca. 800°C. Overall reaction presented in equation 5.

No significant material loss was expected from this step. No data was available concerning emissions. To estimate energy requirements, we modeled the calcination in a chamber furnace. We started with a 8300 litre Nabertherm W83000/85A chamber furnace, with maximum temperature of 850°C and a 200 kW connected load (44). At 800°C, we estimated that a 100 kW half-load is necessary to maintain furnace at 800°C, and 12.5 kW for 405°C. We further assumed a coefficient of utilization of 33%. With these parameters, ca. 1 MJ is required per litre processed. From the molar ratios and densities of the chemicals in equation 5, we estimate a volume of inputs of 0.55 l per kg of final product, and thus an energy requirement of 0.55 MJ·kg⁻¹. Energy requirements for grinding and pelleting were ignored. The process inventory was compiled in Table S8.

Table S8: Inventories for the production of 1 kg of $\text{LiNi}_{0.4}\text{Co}_{0.2}\text{Mn}_{0.4}\text{O}_2$.

Process	Amount	Sub-Inventory
Functional Unit Output		
Lithium nickel cobalt manganese oxide ($\text{LiNi}_{0.4}\text{Co}_{0.2}\text{Mn}_{0.4}\text{O}_2$) (kg)	1	
Material Requirements		
Lithium hydroxide (LiOH) (kg)	0.25	
Nickel cobalt manganese hydroxide ($\text{Ni}_{0.4}\text{Co}_{0.2}\text{Mn}_{0.4}(\text{OH})_2$) (kg)	0.95	Section 7.1
Energy and Processing Requirements		
Heat, unspecified, in chemical plant (MJ)	0.55	
Transport Requirements		
Freight rail transport (tkm)	0.72	
Lorry >16t (tkm)	0.12	
Infrastructure Requirements		
Chemical plant, organics (unit)	4.6×10^{-10}	
Emissions		
Waste heat (MJ)	5.5	

4.7 Production of electrode substrates for lithium ion battery

The electrode paste rests on a thin (ca. 15-20 μm) metal foil, which serves as a physical support and as a current collector. Aluminum foil is used for the positive electrode, while for the negative electrode copper is preferred (4, 30).

No data was available concerning the actual foil fabrication process. For this inventory, “sheet rolling” process was used as a proxy. The inventory may be found in Table S9.

Table S9: Inventories for the production of 1 kg of electrode substrate for Li-ion battery (positive or negative)

Process	Amount
Functional Unit Output	
Li-ion electrode substrate (positive or negative), at plant (kg)	1
Material Requirements	
Positive electrode: Aluminium, production mix (kg)	
Negative electrode: Copper, primary, GLO (kg)	1
Energy and Processing Requirements	
Positive electrode: Sheet rolling, aluminum (kg)	
Negative electrode: Sheet rolling, copper (kg)	1
Transport Requirements	
Freight rail transport (tkm)	0.2
Lorry >16t (tkm)	0.1
Infrastructure Requirements	
Metal working factory (unit)	4.6×10^{-10}

GLO = Global average

4.8 Production of battery management system

Li-ion cells require control circuitry to prevent situations of over-charging or over-discharging. Contrarily to NiMH cells and other aqueous electrolyte based chemistries, Li-ion cells are devoid of any inherent stabilization mechanism, and thus require active external control (4). These include voltage or temperature cut-off control circuits, bypass circuits, fuses, positive coefficient devices (13, 30).

The mass breakdown by Schexnayder et al. (7), estimated that the battery management system (BMS) represented ca. 4% of the battery mass. Circuit boards and wires each constituted about half of this mass. We feel that this may overestimate the relative importance of the BMS. Rather, our best estimate assumes the BMS to represent ca. 3% relative to the whole battery pack, with integrated circuits accounting for roughly 10% of of the BMS mass. Copper wires (both for internal and external cabling) were assumed to represent half of the BMS mass, and a stainless steel container the remainder (Table S10).

Table S10: Production of 1 kg of battery management system for Li-ion battery

Process	Amount
Functional Unit Output	
Battery management system for Li-ion battery (kg)	1
Material Requirements	
Integrated circuit, logic type, at plant (kg)	0.1
Copper, primary, at refinery (kg)	0.5
Chromium steel 18/8 (kg)	0.4
Energy and Processing Requirements	
Wire drawing, cooper (kg)	0.5
Sheet rolling, steel (kg)	0.4
Transport Requirements	
Freight rail transport (tkm)	0.2
Lorry >16t (tkm)	0.1
Infrastructure Requirements	
Plastic processing factory (unit)	2.3×10^{-10}

5 Inventory of NiMH battery production

5.1 Manufacture of NiMH Battery and subcomponents

The assembly of NiMH batteries resembles that of Li-ion batteries. For both the negative and the positive electrodes, the electrode paste is applied in the porous substrate. The slurry is dried and roll pressed (8). The electrodes are then wound together with the separator, inserted in the cell container and put in contact with the electrolyte (11). After testing, the cells are combined in modules and battery packs.

The inventoried material requirements are based on the mass shares of the components of the modeled NiMH (see Table S1). Energy requirements were taken from Rydh and Sandén (26), as

discussed in Sections 8.2 and 8.3, below. Direct water, transport, and infrastructure inputs were taken Hirschier et al. (31). The process inventory was compiled in Table S11.

Table S11: NiMH battery assembly

Parameter	Amount	Sub-Inventory
Functional Unit Output		
NiMH battery, assembled (kg)		
Material Requirements		
Positive electrode paste for NiMH battery (kg)	0.20	Section 5.3
Negative electrode paste for NiMH battery (kg)	0.17	Section 5.2
Positive electrode substrate for NiMH battery (kg)	0.13	Section 5.5
Negative electrode substrate for NiMH battery (kg)	0.11	Section 5.5
Electrolyte for NiMH battery (kg)	0.09	Section 5.4
Separator (kg)	0.04	Section 6.2
Cell container, tab and terminals (kg)	0.10	Section 6.1
Module and Battery Container (kg)	0.17	Section 6.3
Control circuitry (kg)	-	
Water, decarbonated	183	
Processing and Energy requirements		
Electricity, medium voltage, UCTE, at grid (MJ)	31	
Heat, light fuel oil, at industrial furnace 1MW	3.4	
Heat, natural gas, industrial furnace low-NO _x > 100 kW	26	
Transport Requirements		
Freight rail transport (tkm)	0.10	
Lorry >16t (tkm)	0.03	
Infrastructure		
Facility, precious metal refinery (SE) (unit)	7.8x10 ⁻⁸	
Emissions		
Waste heat (MJ)	31	

SE = Sweden

5.2 Production of Negative Electrode Paste for NiMH

The paste is composed of the electrochemically active AB₅ alloy, a binder, and other additives. The LaNi₅ compound is the starting point of AB₅ alloys (45). In practice however, lanthanum is often substituted by lanthanum-rich mischmetal (Lm), and a fraction of the nickel is often replaced by other metals (Co, Ce, Mn, Al, etc.) (8, 46). Different alloying techniques have been reported, including mechanical alloying (47), electric arc fusion (48), and radio-frequency induction fusion (49), all under argon atmosphere. To yield small crystal grain sizes, the fusion step is followed by rapid cooling in plate-like casting, gas atomization or melt-spinning (45, 49). The resulting alloy is then pulverized, either mechanically or by hydrogen absorption-desorption cycles (48), and mixed with the binder and additives. Commonly used binders include hydroxylpropylmethyl cellulose (HPMC), carboxymethyl cellulose (CMC) and polytetrafluoroethylene (PTFE) (50). Carbon black is commonly added to increase conductivity (8).

Here, we model an electrode paste containing 3% CMC, 3% PTFE, and 2% carbon black, in accordance with the recommendations of Yang et al. (50) and Ying et al. (8). The rest was made up of mischmetal and nickel, in stoichiometric 1:5 molar ratios. Electric arc fusion was assumed, with the average electricity mix of the UCTE. The electricity requirement was based on the thermodynamic melting of nickel and lanthanum (51). Hydrogen requirements for the absorption-desorption pulverisation were based estimate by Hischier et al. (31). Due to lack of data, no material loss or emissions other than hydrogen and heat were compiled. Energy requirements for grinding and mixing are not expected to be important and were ignored. Requirements of argon atmosphere were omitted due to lack of data. The detailed inventory may be found in Table S12.

Table S12: Inventory for the production of 1 kg negative electrode paste for AB₅ NiMH battery

Process	Amount
Functional Unit Output	
Negative electrode paste for AB ₅ NiMH (kg)	1
Material Requirements	
Mischmetal (kg)	0.30
Nickel (kg)	0.62
Carboxymethyl cellulose (CMC) (kg)	0.03
Polytetrafluoroethylene (PTFE) (kg)	0.03
Carbon black (kg)	0.02
Liquid Hydrogen (kg)	0.92
Energy and Processing Requirements	
Electricity, high voltage, UCTE production mix (MJ)	0.75
Transport Requirements	
Freight rail transport, European conditions (tkm)	0.6
Lorry >16t, European conditions (tkm)	0.1
Infrastructure Requirements	
Chemical plant (unit)	4x10 ⁻¹⁰
Emissions	
Hydrogen gas (kg)	0.92
Waste heat (MJ)	0.75

5.3 Production of Positive Electrode Paste for NiMH

The positive electrode material for NiMH is composed predominantly (ca. 85%) of nickel II hydroxide (Ni(OH)₂). It is worth noting that nickel is maintained in its oxidized form, and never goes through the energy-intensive process of being reduced to its metallic form. Nickel powder, cobalt hydroxide (Co(OH)₂), zinc, graphite or carbon black are often added for performance enhancement. Either carboxymethyl cellulose (CMC) or polytetrafluoroethylene (PTFE) are used as binders (8, 52-54). The paste is achieved by simple mixing, with minor energy or processing requirements.

For the purpose of this inventory, a slurry composition of 85% Ni(OH)₂, 10% carbon black, 2.5% PTFE and 2.5% CMC was assumed, based on a compromise between the protocols of Liu & Yu (52) and Ying et al. (8). Direct energy requirements for electrode paste production are negligible. No

infrastructure use was allocated to this process, as it would be performed on-site at the battery assembly plant. This process being a simple mixing step, no material loss or emissions are expected. The detailed inventory may be found in Table S13.

Table S13: Inventory for the production of 1 kg of positive electrode material for NiMH battery.

Process	Amount	Sub-Inventory
Functional Unit Output		
Positive Electrode Material for NiMH, at plant (kg)	1	
Material Requirements		
Nickel hydroxide (Ni(OH)_2) (kg)	0.85	Section 7.1
Carbon black, GLO (kg)	0.10	
Carboxymethyl cellulose (CMC) (kg)	0.025	
Polytetrafluoroethylene (PTFE) (kg)	0.025	
Transport Requirements		
Freight rail transport (tkm)	0.6	
Lorry >16t (tkm)	0.1	

GLO = Global average

5.4 Production of electrolyte for NiMH battery

NiMH batteries rely on a basic aqueous solutions for electrolytes. Based on Ying et al. (8), concentrations of $6 \text{ mol} \cdot \text{L}^{-1}$ of potassium hydroxide (KOH) and $1 \text{ mol} \cdot \text{L}^{-1}$ of lithium hydroxide (LiOH) were assumed. The different masses were calculated using a solution density of $1.3 \text{ kg} \cdot \text{L}^{-1}$ (55). The deionization of water and the salt dissolution were assumed to be performed on-site at the battery assembly plant, and thus no infrastructure requirements were assigned to this process. No material losses or direct emissions are expected. The detailed inventory may be found in Table S14.

Table S14: Inventory for the production of 1 kg of electrolyte for NiMH battery.

Process	Amount
Functional Unit Output	
Electrolyte for NiMH Battery (kg)	1
Material Requirements	
Potassium hydroxide (KOH) (kg)	0.26
Lithium hydroxide (LiOH) (kg)	0.02
Deionized water (kg)	0.72
Transport Requirements	
Freight rail transport (tkm)	0.17
Lorry >16t (tkm)	0.03

5.5 Production of NiMH electrode substrate

Typical substrate materials for NiMH negative electrodes include nickel-plated perforated steel sheets, nickel mesh, nickel foam or nickel fiber mats (56). Copper screens were also reported (57). For the positive electrode, the standard option seems to be nickel foam (8, 52-54, 58). For simplicity, a nickel foam substrate was assumed for both electrodes of the NiMH.

Nickel foam is generally produced by electrodeposition of nickel ions (e.g. NiSO_4) on polyurethane (PUR) foam. To ensure conductivity, the foam is first covered by a layer of a carbon-based colloid or chemically plated nickel. After the electroplating is complete, the polymer backbone is burned off in air (600°C, 4 minutes) and the nickel foam is sintered (980°C for 40 min) in reductive atmosphere (59).

The relative amounts of nickel and polyurethane were estimated based on the nickel foam density (310 kg · m⁻³) reported by Okuno et al. (53) and by assuming a polyurethane density of 6 kg · m⁻³. As little information could be found on the emissions and the energy requirements of nickel ion electroplating, metallic nickel was used as a proxy. The energy requirement to heat the nickel mesh to 600°C was calculated assuming thermodynamic heating of nickel (51), neglecting both heat losses and any energy released by polyurethane combustion. The energy requirements of the nickel foam sintering step were estimated based on the iron sintering process reported in Ecoinvent (60), as the latter has comparable temperature requirements (ca. 1150°C) (61). No other aspect of the sintering was modeled. For the emissions resulting from the burning off of polyurethane, polyurethane combustion in a municipal incinerator was used as a proxy. Heat wastes were based on heat requirements. Any other emission was ignored. It is assumed that nickel foam production is outsourced to specialized metallurgy companies by the battery manufacturer (62). The detailed inventory may be found in Table S15.

Table S15: Inventory for the production of 1 kg of nickel foam electrode substrate for NiMH battery.

Process	Amount
Functional Unit Output	
NiMH nickel foam electrode substrate, at plant (kg)	1
Material Requirements	
Nickel, 99.5%, GLO [proxy for electroplated NiSO_4] (kg)	1
Polyurethane, flexible foam (kg)	0.019
Energy and Processing Requirements	
Heat, unspecified, in chemical plant [burn-off polyurethane] (MJ)	0.078
Heat, unspecified, in chemical plant [sinter] (MJ)	1.5
Transport Requirements	
Freight rail transport (tkm)	0.61
Lorry >16t (tkm)	0.20
Infrastructure Requirements	
Chemical plant, organics (unit)	4.0x10 ⁻¹⁰
Emissions	
Disposal of Polyurethane to municipal incinerator, [proxy for combustion], CH (kg)	0.019
Waste heat (MJ)	1.58

GLO = Global average

6 Inventory of common components production

6.1 Production of cell containers

The cell containers for lithium-ion batteries will generally be made of aluminum, though stainless steel is sometimes used (4). For NiMH, stainless steel is the preferred option (7), possibly due to its higher resistance to corrosion attack from the basic electrolyte (51). Having no specific data on the container production, this process was inventoried with metal sheet rolling as a proxy. The detailed inventory may be found in Table S16.

Table S16: Inventories for the production of 1 kg of cell containers for Li-ion or NiMH.

Process	Amount
Functional Unit Output	
Cell container (Li-ion or NiMH), at plant (kg)	1
Material Requirements	
Cell container, li-ion: Aluminium, production mix (kg)	1
Cell container, NiMH: Chromium steel 18/8 (kg)	
Energy and Processing Requirements	
Cell container, li-ion: Sheet rolling, aluminum (kg)	1
Cell container, NiMH: Sheet rolling, steel (kg)	
Transport Requirements	
Freight rail transport (tkm)	0.2
Lorry >16t (tkm)	0.1
Infrastructure Requirements	
Metal working factory (unit)	4.6x10 ⁻¹⁰

6.2 Production of separator

The fundamental role of the separator is to prevent the two electrodes from touching, while letting electrons in the electrolyte flow with as little resistance as possible. Li-ion and NiMH separators are both typically made of porous polymer. For NiMH, materials such as non-woven polyamide (56), sulphonated polypropylene fabric (53), non-woven PVC cloth (58), polypropylene (PP) and polyethylene (PE) (63) have been reported. Similarly, Li-ion cells generally rely on polypropylene and polyethylene (4, 30, 64). Other materials being researched include polyacrylonitrile (PAN) and ceramic composite based non-woven polyolefins, along with hydrophilic SiO₂ powder (13).

In this study, we modeled in the same manner the separator for both Li-ion and NiMH batteries. It was assumed to be composed of PP and PE, in equal amounts. Injection molding was used as a proxy to model the processing of the materials. No material losses were accounted for.

Table S17: Production of 1 kg of separator for Li-ion or NiMH batteries

Process	Amount
Functional Unit Output	
Separator material for Li-ion or NiMH (kg)	1
Material Requirements	
Polyethylene, LDPE granulate, at plant (kg)	0.5
Polypropylene, granulate, at plant (kg)	0.5
Energy and Processing Requirements	
Injection moulding (kg)	
Transport Requirements	
Freight rail transport (tkm)	0.2
Lorry >16t (tkm)	0.1
Infrastructure Requirements	
Plastic processing factory	7.4×10^{-10}

6.3 Production of module and battery packing

Multiple cells are combined together as modules, which are in turn combined in battery packs. Plastics are usually the dominant material in module and battery packs, since they are resistant to corrosion, inexpensive, and light (4). For this inventory, we combined as one entity the packing for the modules and the battery pack, and used polyethylene terephthalate (PET) for both. The inventory for this process was compiled in Table S18.

Table S18: Production of 1 kg of module and battery packing

Process	Amount
Functional Unit Output	
Module and battery packing	1
Material Requirements	
Polyethylene terephthalate	1
Energy and Processing Requirements	
Injection moulding (kg)	1
Transport Requirements	
Freight rail transport (tkm)	0.2
Lorry >16t (tkm)	0.1
Infrastructure Requirements	
Plastic processing factory	7.4×10^{-10}

7 Inventory intermediate materials production

7.1 Production of transition metal hydroxides

Nickel hydroxide ($\text{Ni}(\text{OH})_2$) and $\text{Ni}_{0.4}\text{Co}_{0.2}\text{Mn}_{0.4}(\text{OH})_2$ are starting materials of the positive electrode pastes of NiMH and NCM Li-ion batteries, respectively. Their production process consists in the precipitation of the metal hydroxides from an aqueous solution of the metal salts by reaction with a

strong base (12, 15, 65). The products are recuperated by filtration and dried at low temperature (ca. 120°C) in air. For this inventory, the sulphate salt of each metal was used in combination with sodium hydroxide (eq. 6 and 7). This simple mixture and precipitation step is not expected to have significant energy requirements. As these metal hydroxides are virtually insoluble in alkaline solutions (55), no product loss was accounted for.

Table S19: Inventories for the production of 1 kg of Ni(OH)₂.

Process	Amount	Sub-Inventory
Functional Unit Output		
Nickel hydroxide (Ni(OH) ₂) (kg)	1	
Material Requirements		
Nickel sulphate (NiSO ₄) (kg)	1.67	Section 7.2
Sodium hydroxide (NaOH) (kg)	0.86	
Transport Requirements		
Freight rail transport (tkm)	1.5	
Lorry >16t (tkm)	0.25	
Infrastructure Requirements		
Chemical plant, organics (unit)	4.6x10 ⁻¹⁰	
Emissions		
Sodium sulphate (Na ₂ SO ₄) (kg)	1.5	

Table S20: Inventories for the production of 1 kg of Ni_{0.4}Co_{0.2}Mn_{0.4}(OH)₂.

Process	Amount	Sub-Inventory
Functional Unit Output		
Nickel cobalt manganese hydroxide (Ni _{0.4} Co _{0.2} Mn _{0.4} (OH) ₂) (kg)	1	
Material Requirements		
Nickel sulphate (NiSO ₄) (kg)	0.68	Section 7.2
Cobalt sulphate (CoSO ₄) (kg)	0.34	Section 7.2
Manganese sulphate (MnSO ₄) (kg)	0.66	Section 7.3
Sodium hydroxide (NaOH) (kg)	0.88	
Transport Requirements		
Freight rail transport (tkm)	1.5	
Lorry >16t (tkm)	0.26	
Infrastructure Requirements		
Chemical plant, organics (unit)	4.6x10 ⁻¹⁰	
Emissions		
Sodium sulphate (Na ₂ SO ₄) (kg)	1.5	

7.2 Production of NiSO_4 and CoSO_4

Most of the nickel sulphate on the market is a by-product of electrolytic copper refining (65). Similarly, cobalt sulphate is frequently acquired as a by-product of nickel and copper leaching (e.g. Gécamines process) (66). These three metals are mined jointly in sulfidic ores (67). Both NiSO_4 and CoSO_4 are typically intermediates in the process of refining metallic nickel and cobalt by electrowinning. They are produced by sulphuric acid leaching of ore concentrates or sulfidic matte. As they have not yet undergone the energy intensive reduction step to the neutral metal, nickel and cobalt sulphates have a lower energy requirement than their neutral metallic counterparts.

No inventory could be found detailing the production of NiSO_4 or CoSO_4 . Their production requirements were rather approximated by modifying the inventories for primary nickel and cobalt metals in Ecoinvent. By removing any reduction, carbonyl reaction or electrorefining step, these modified processes thus conceptually yield metal ions rather than neutral metal. This approximation is certainly crude, but constitutes an improvement relative to using metals as a direct proxy for metal sulphate salts.

The Ecoinvent inventory of nickel production is a relatively detailed combination of five commonly used industrial paths (60). These paths were separated, and the steps refining nickel beyond the NiSO_4 intermediate were eliminated. All requirements pertaining to ore mining, beneficiation, drying, roasting, and primary smelting were conserved, as were matte conversion and separation of co-products (both wet and dry). All requirements linked to primary refining, nickel refining, reduction, and carbonyl reaction were removed. This new process thus constitutes an “intermediate process”, with unrefined metal ions as output. No information allowed for a disaggregation of the emissions and the waste disposals between the pre-reduction and the reduction phase. Consequently, emission and waste disposal requirements were not modified.

Evidently, nickel ions must undergo processing in going from crude ionic solution to pure NiSO_4 crystals. These would include matte leaching in the case of dry co-product separation, crystallization, and possibly recrystallization. Relative to the whole metallurgy process, these processes are not expected to have high energy requirements. They were not accounted for in this inventory due to lack of data. The sulphuric acid requirements for NiSO_4 production were ignored. The production of H_2SO_4 as a by-product of sulfidic ore metallurgy far outweighs the leaching requirements, and Ecoinvent does not account quantitatively for this output.

As recognized by Hischier (68), the process description for cobalt production in Ecoinvent is not as detailed and exhaustive as that of nickel. Nevertheless, it is clearly stated which requirements are made necessary by the reduction step. These were removed from the inventory of CoSO_4 . Emissions, waste disposal and sulphuric acid requirements were dealt with in the same way as for NiSO_4 .

Table S21: Inventories for the production of 1 kg of NiSO₄, produced by modifying the Ecoinvent inventory for class I nickel.

Process	Modification from metallic nickel in Ecoinvent	Inventory for production of NiSO ₄
Functional Unit Output	Modifications for 379.3 g of Ni ⁰ metal to Ni ²⁺	1 kg NiSO ₄ (379.3 g Ni ²⁺)
Material Requirements		
Ammonia, liquid, at regional storehouse (kg)	-	0.032
Chemicals inorganic (kg)	-	0.023
Chemicals organic (kg)	-	0.0068
Hydrogen cyanide (kg)	-	0.0011
Hydrogen liquid (kg)	-0.0017	-
Limestone, milled, packed (kg)	-	0.73
Portland calcareous cement (CH) (kg)	-	1.0
Sand, at mine (CH) (kg)	-	13
Silica sand (kg)	-	0.72
Energy and Processing Requirements		
Blasting (kg)	-	0.046
Diesel, burned in building machine (GLO) (MJ)	-	3.1
Electricity, high voltage, UCTE (MJ)	-1.0	4.1
Electricity, hydropower, at run-of-river (MJ)	-1.5	10.5
Electricity, medium voltage, UCTE (MJ)	-	1.7
Heat, hard coal, industrial furnace 1-10 MW (MJ)	-	0.71
Heavy fuel oil, burned in industrial furnace 1 MW (MJ)	-0.46	8.1
Natural gas, burned in industrial furnace > 100 kW (MJ)	-2.0	3.5
Transport Requirements		
Lorry >16t (tkm)	-	0.68
Infrastructure Requirements		
Non-ferrous metal mine, underground (GLO) (unit)	-	1.5x10 ⁻⁹
Non-ferrous metal smelter (GLO) (unit)	-	1.3x10 ⁻¹¹
Aluminium hydroxide plant (unit)	-	2.5x10 ⁻¹⁰
Conveyor belt (m ³)	-	1.2x10 ⁻⁶
Waste Disposal		
Disposal, nickel smelter slag, 0% water, residual material landfill (CH) (kg)	-	3.6
Disposal, sulfidic tailings, off-site (GLO) (kg)	-	27

CH = Switzerland, GLO = Global average

Table S22: Inventories for the production of 1 kg of CoSO₄, produced by modifying the Ecoinvent inventory for primary cobalt

Process	Modification from metallic cobalt in Ecoinvent	Inventory for production of CoSO ₄
Functional Unit Output		
	Modifications for 380.2 g of Co ⁰ metal to Co ²⁺	1 kg CoSO ₄ (380.2 g Co ²⁺)
Material Requirements		
Carbon monoxide (kg)	- 0.11	-
Chemicals inorganic, at plant (GLO) (kg)	-	0.032
Chemicals organic, at plant (GLO) (kg)	-	0.010
Hydrogen cyanide, at plant (kg)	-	0.0015
Hydrogen, liquid, at plant (kg)	- 0.0079	-
Limestone, milled, packed, at plant (CH) (kg)	-	0.019
Portland calcareous cement, at plant (CH) (kg)	-	1.4
Sand, at mine (CH) (kg)	-	17
Energy and Processing Requirements		
Blasting (kg)	- 0.11	0.063
Diesel, burned in building machine (GLO) (MJ)	-	4.6
Electricity, medium voltage, production UCTE (MJ)	-	6.4
Heat, natural gas, at industrial furnace >100 kW (MJ)	-0.76	-
Transport Requirements	-	
Lorry >16 t (tkm)	-	0.94
Infrastructure Requirements		
Aluminium hydroxide, plant (unit)	-	3.4x10 ⁻¹⁰
Conveyor belt, at plant (m ³)	-	1.6x10 ⁻⁶
Non-ferrous metal mine, underground (GLO) (unit)	-	2.1x10 ⁻⁹
Waste Disposal		
Disposal, nickel smelter slag, 0% water, residual material landfill (CH) (kg)		13
Disposal, sulfidic tailings, off-site (GLO) (kg)		25

CH = Switzerland, GLO = Global average

Table S23: Direct emissions for the production of 1 kg of NiSO₄ and 1kg of CoSO₄, based on Ecoinvent emission inventories of metallic nickel and cobalt production

Emissions	Compartment	NiSO ₄	CoSO ₄
Nickel, 1.13% in sulphide, Ni 0.76% and Cu 0.76% in crude ore, in ground (kg)	Raw	4.8x10 ⁻¹	-
Cobalt, in ground (kg)	Raw	-	5.0x10 ⁻¹
Water, river (m ³)	Raw	1.1x10 ⁻²	1.4x10 ⁻²
Water, well, in ground (m ³)	Raw	6.1x10 ⁻²	8.4x10 ⁻²
Aluminum (kg)	Air	5.6x10 ⁻⁴	-
Arsenic (kg)	Air	2.0x10 ⁻⁶	-
Calcium (kg)	Air	3.9x10 ⁻⁴	-
Carbon dioxide, fossil (kg)	Air	3.2x10 ⁻¹	-
Carbon disulphide (kg)	Air	3.0x10 ⁻³	4.2x10 ⁻³
Cobalt (kg)	Air	4.2x10 ⁻⁴	-
Copper (kg)	Air	1.3x10 ⁻⁴	-
Dioxins, measured as 2,3,7,8-tetrachlorodibenzo-p-dioxin (kg)	Air	3.5x10 ⁻¹²	-
Heat, waste (MJ)	Air	2.0x10 ¹	6.4x10 ⁰
Lead (kg)	Air	1.2x10 ⁻⁵	-
Magnesium (kg)	Air	3.3x10 ⁻⁴	-
Nickel (kg)	Air	1.5x10 ⁻⁴	-
NM VOC, non-methane volatile organic compounds, unspecified origin (kg)	Air	6.9x10 ⁻⁵	-
Particulates, < 2.5 um (kg)	Air	5.7x10 ⁻³	7.5x10 ⁻⁴
Particulates, > 10 um (kg)	Air	5.8x10 ⁻⁴	7.7x10 ⁻³
Particulates, > 2.5 um, and < 10um (kg)	Air	5.0x10 ⁻³	6.7x10 ⁻³
Silver (kg)	Air	4.8x10 ⁻⁸	-
Sulphur dioxide (kg)	Air	5.1x10 ⁻¹	-
Tin (kg)	Air	2.3x10 ⁻⁶	-
Zinc (kg)	Air	3.5x10 ⁻⁵	-
Aluminium (kg)	Water	5.2x10 ⁻⁶	7.2x10 ⁻⁶
Arsenic, ion (kg)	Water	2.6x10 ⁻⁷	2.5x10 ⁻⁷
BOD5, Biological Oxygen Demand (kg)	Water	6.3x10 ⁻⁴	-
Cadmium, ion (kg)	Water	3.1x10 ⁻⁸	2.6x10 ⁻⁸
Calcium, ion (kg)	Water	1.3x10 ⁻²	5.7x10 ⁻²
Calcium, ion (kg)	Water	2.9x10 ⁻²	-
Chromium, ion (kg)	Water	1.6x10 ⁻⁷	4.6x10 ⁻⁸
Cobalt (kg)	Water	4.7x10 ⁻⁸	6.5x10 ⁻⁸
COD, Chemical Oxygen Demand (kg)	Water	6.3x10 ⁻⁴	8.7x10 ⁻⁴
Copper, ion (kg)	Water	7.1x10 ⁻⁷	6.7x10 ⁻⁷
Cyanide (kg)	Water	1.1x10 ⁻⁴	1.6x10 ⁻⁴
DOC, Dissolved Organic Carbon (kg)	Water	2.5x10 ⁻⁴	-
Iron, ion (kg)	Water	1.8x10 ⁻⁵	2.4x10 ⁻⁵
Lead (kg)	Water	2.4x10 ⁻⁷	2.3x10 ⁻⁷
Manganese (kg)	Water	1.5x10 ⁻⁶	2.1x10 ⁻⁶
Mercury (kg)	Water	3.5x10 ⁻⁹	3.2x10 ⁻⁹
Nickel, ion (kg)	Water	1.6x10 ⁻⁶	2.0x10 ⁻⁶
Nitrogen, organic bound (kg)	Water	1.4x10 ⁻³	-
Nitrogen (kg)	Water	-	1.9x10 ⁻³
Solved solids (kg)	Water	3.1x10 ⁻⁴	4.3x10 ⁻⁴
Sulphate (kg)	Water	1.4x10 ⁻¹	2.0x10 ⁻¹
Tin, ion (kg)	Water	1.2x10 ⁻⁷	-
TOC, Total Organic Carbon (kg)	Water	2.5x10 ⁻⁴	-
Zinc, ion (kg)	Water	5.0x10 ⁻⁶	6.4x10 ⁻⁶

7.3 Production of $MnSO_4$

Similarly to $NiSO_4$ and $CoSO_4$, manganese II sulphate ($MnSO_4$) is an intermediate in the electrolytic (hydrometallurgy) route to metallic manganese production (69). Manganese ore is typically insoluble and predominantly in +4 oxidation state (e.g. MnO_2). Manganese carbonates constitute an exception, and can be leached directly. In other cases, the ore is calcinated at ca. 850-1000°C under reducing atmosphere to yield the manganese II oxide (MnO) intermediate. Anthracite, coal, charcoal, hydrocarbon oils, natural gas, coal gas and liquefied petroleum gas are used in different proportions as sources of carbon, which is the reducing reagent of choice. Following reduction, MnO is then finely ground and leached with a 2-5% H_2SO_4 solution. Other metals are removed from solution by air oxidation (iron), pH manipulations, and soluble sulphide dissolution. Manganese sulphate concentrations in solution typically reaches 10% (69). In the metallurgy route, the manganese would then be reduced to its metallic form by cathodic deposition. To obtain the salt intermediate, the manganese sulphate must be crystallized out of solution, and possibly recrystallized.

No inventory could be found for the production of $MnSO_4$. The inventory for manganese metal production in Ecoinvent could not be used as a starting point. As recognized by Classen et al. (60), the precision and completeness of this process description is very low. In fact, the electricity requirement for the hydrolytic reduction of manganese ions is the only significant distinction between this process and the manganese ore concentrate; all material requirements and emissions being omitted.

Here we provide a crude model of $MnSO_4$ production. Though limited and based on estimations, it represents nonetheless an improvement relative to using manganese concentrate or manganese metal as proxies. Manganese concentrate was assumed to contain 42% manganese, consistent with world average concentration (60). A leaching efficiency of 90% is consistent with current practices (70). We further assume a 90% crystallization efficiency. The fuel requirements for the reductive calcination of manganese IV dioxide were estimated to equal that of iron sintering, which operates at similar temperatures. The grinding energy requirements were of 20 kWh per metric ton of processed ore (60). Sulphuric acid use was determined stoichiometrically. Energy requirements for crystallization, which should be relatively unimportant, were not modeled due to lack of data. Direct emissions, which may be substantial, were omitted for the same reasons.

Table S24: Inventory for the production of 1 kg of MnSO₄

Process	Amount
Functional Unit Output	
Manganese sulphate, at plant (MnSO ₄) (kg)	1
Material Requirements	
Manganese concentrate, at beneficiation (GLO) (kg)	1.1
Sulphuric acid, liquid, at plant (kg)	0.65
Energy and Processing Requirements	
Natural gas, high pressure, at consumer (MJ)	0.036
Hard coal coke, at plant (MJ)	1.43
Electricity, medium voltage, production UCTE, at grid (MJ)	0.077
Transport Requirements	
Freight rail transport, European conditions (tkm)	0.39
Lorry >16 t (tkm)	0.06
Infrastructure Requirements	
Non-ferrous metal mine, underground (GLO) (unit)	1.6x10 ⁻¹⁴
Aluminium hydroxide plant (unit)	2.4x10 ⁻¹⁰
Waste and Emissions	
Disposal, non-sulfidic tailings, off-site (GLO) (kg)	0.71
Waste heat, to air (MJ)	1.5

GLO = Global average

8 Energy requirements of production phase

8.1 Energy scoping

While material requirement estimates could generally be guided by dismantling reports or mass balance considerations, quantifying energy requirements in a process-wise manner proved challenging. No public report could be found in which a battery producer directly disclosed its energy requirements in a sufficiently detailed manner. This lead us to employ a top-down approach, using reported industry overall energy requirements, as reviewed in Table S25.

Amongst the different estimates, we considered the values reported by Rydh and Sanden (26) to be most credible, partly because Carl Johan Rydh has worked for SAFT (battery company), partly because their publication focuses precisely on energy use, and partly because their estimates have been used in other energy and LCA publications, e.g. Samaras and Meisterling (71). They claim that their reported “Manufacture” energy requirement covers all requirements from virgin material to final product.

Table S25: Review of overall energy requirements reported for battery production, all expressed as MJ per kg of battery

Type	Production Year	Energy Requirements (MJ·kg ⁻¹)		Covers		Notes
		Primary	Absolute	Materials	Manufacture	
Li-ion	a < 1999		El : 54.6	-	X	Only covers electricity
	b 2002-2003		288 (El: 148, Gas: 123, Oil:16)	-	X	For laptop use
	c < 2003	96-144*		-	X	For static application
	c < 2003	149-224*		X	X	For static application
	d < 2009		1.40		X	
	d < 2009	104		X	X	Whole life cycle
NiMH	e 1996		10.3 (El: 1.96, Gas: 8.35)	-	X	
	c < 2003	74-139**		-	X	For static application
	c < 2003	128-241**		X	X	For static application
	b 2002-2003		144 (El: 77, Gas:59, Oil: 8)	-	X	Battery for laptop use

* 75% of primary energy for electricity production, with assumed conversion efficiency to electricity of 35%

** 68% of primary energy for electricity production with assumed conversion efficiency to electricity of 35%

a Almemark et al. (72); based on Japanese CRIEPI data

b Hischier et al. (31); Ecoinvent 2.1, based on Maxell 2003 environmental report

c Rydh and Sandén (26); d Notter et al. (73); e Rantik (74);

8.2 Energy Mix

Rydh and Sandén (26) report that 75% of the primary energy requirements of battery manufacture are attributable to electricity consumption, with a 35% conversion efficiency from primary fuel to electricity. We assume that the remainder 25% of the primary energy requirements are fulfilled directly by fossil fuel combustion for heat production or in machinery, with nearly 100% “conversion” efficiency. Thus, in terms of “direct” energy requirements, electricity and fossil fuel would each fulfill roughly 50% of the energy bill. This energy mix is in agreement with overall reported figures reported by Saft (75) and Maxell (76) industries. For this inventory, we use the following energy mix for direct inputs to the battery manufacturing process: 51.7% electricity, 42.7% heat from natural gas combustion and 5.5% heat from light fuel oil. This ratio was inspired by the Maxell (76) environmental report. The electricity mix was taken to be the average mix of the Union for the Coordination of Transmission of Electricity (UCTE).

8.3 Energy inventory

As mentioned above, we took a top-down approach to cover all energy requirements related to manufacture of the battery. From this overall total, we then tried to bring a more detailed perspective by “separating out” the known energy requirements for specific battery manufacturing processes.

For production from cradle to gate, using virgin materials, Rydh and Sandén (26) estimated total primary fuel requirements of 1.87 MJ·kWh⁻¹ of Li-ion capacity, and 3.7 MJ·kWh⁻¹ of NiMH capacity. Of this total, 1.2 MJ·kWh⁻¹ and 2.1 MJ·kWh⁻¹ were dedicated to “manufacturing” of Li-ion and NiMH, respectively; the rest being required for virgin material production. The problem remains the concept of “manufacture” is not a very clearly defined system boundary. In particular, it is not explicitly stated at

which level of refinement a process ceases to belong to “material production” and falls over to “manufacturing”. For this paper, we define the modification of any material beyond its elemental or uncomplicated state to belong to “manufacturing”; Rydh and Sandén's “material production” is interpreted as being limited to pure metals, simple plastics, or raw chemicals. We are comforted in this interpretation by a certain number of elements in the Rydh and Sandén study. First, it is an implicit requirement of their model that the production of any non-manufactured material must be possible either by recycling or by production of virgin material, which is certainly not the case for complicated chemicals or components. Secondly, the PhD thesis of Rydh (77) helps put the present energy analysis in context by relating it to other papers. In this thesis, we learn that the energy requirements for material production were based on the grouped LCI data that lead to the publication by Rydh and Sun (78), which only covers pure or simple materials. In the PhD thesis, it is also emphasized that the energy study in question is partly based on the environmental assessment of vanadium redox and lead-acid batteries by Rydh (79), for which all material requirements (explicitly listed) are either pure metals or simple chemicals. A similar treatment of “raw materials” is observed in the study of NiCd portable batteries by Rydh and Karlstrom (80).

Table S26 summarizes what processes we include in this overall “battery manufacturing” energy use. Thus, for processes included in the overall battery manufacturing (Table S26, first column), any additional energy requirement identified would be separated out of the overall top-down energy requirement. Additional process-specific details were estimated based on published estimates, industrial process modeling, thermodynamic calculations, or the use of proxies (Table S26, last 4 columns).

Table S26: Overview of strategies pursued and assumptions used to quantify the energy requirements for the production of the different battery sub-components and materials.

Process	Part of the top-down overall “battery manufacturing”	Additional process-wise information for direct energy requirements?			
		Estimate in literature	Use model or thermodynamic calculations	Use of Proxy	No*
Production of positive electrode pastes for lithium ion battery (NCM or LFP)	yes				X
Production of negative electrode paste of lithium ion battery (NCM or LFP)	yes		X		
Production of electrolyte for Li-ion battery	yes				X
Production of LiFePO ₄	yes		X		
Production of LiNi _{0.4} Co _{0.2} Mn _{0.4} O ₂	yes		X		
Production of electrode substrates for lithium ion battery	yes			X	
Production of transition metal hydroxides	yes				X
Production of battery management system	yes			X	
Production of Negative Electrode Paste for NiMH	yes		X		
Production of Positive Electrode Paste for NiMH	yes				X
Production of electrolyte for NiMH battery	yes				X
Production of NiMH electrode substrate	yes			X	
Production of cell containers	yes			X	
Production of separator	yes			X	
Production of module and battery packing	yes			X	
Production of NiSO ₄ and CoSO ₄	NO (virgin)		X	X	
Production of MnSO ₄	NO (virgin)				

*Full allocation of process energy requirement to the overall “battery manufacturing”; no further disaggregation.

9 Complete Numerical Results

Total life cycle impacts are presented quantitatively in the main paper. The impacts are also broken down between use-phase and production (Main Paper, Figure 1), and then further split in a component-wise manner (Main Paper, Figure 2), but only graphically. We here present the data underlying these figures (Tables S27, S28, S29). The following impacts are for 50 MJ of energy delivered to the power-train.

Table S27: NiMH life cycle impact for storing and delivering 50 MJ of electrical energy to a power-train, broken down amongst key components

		Battery Use	Battery & Components Manufacture	Positive Electrode Paste	Negative Electrode Paste	Electrolyte	Separator	Cell Container	Module & Battery Casing	Electrode substrates	Electricity Consumed by Battery
GWP ₁₀₀	kg CO ₂ -eq	2.5E-5	7.4E-1	2.6E-1	4.8E-1	5.2E-3	1.4E-2	4.3E-2	7.4E-2	4.4E-1	1.5E+0
FDP	kg oil-eq	8.5E-6	2.4E-1	3.4E-2	1.1E-1	1.7E-3	8.8E-3	1.3E-2	3.9E-2	1.2E-1	4.3E-1
FETP _{inf}	kg 1,4-DCB-eq	7.4E-8	7.1E-3	1.5E-2	2.1E-2	5.0E-5	7.7E-5	3.5E-3	5.4E-4	5.8E-2	2.1E-2
FEP	kg P-eq	4.3E-9	4.9E-4	3.9E-4	6.0E-4	3.2E-6	4.1E-6	2.0E-5	3.2E-5	1.5E-3	1.5E-3
HTP _{inf}	kg 1,4-DCB-eq	3.4E-6	3.3E-1	7.3E-1	9.4E-1	2.5E-3	3.6E-3	3.8E-2	3.0E-2	2.6E+0	9.6E-1
METP _{inf}	kg 1,4-DCB-eq	1.4E-7	7.1E-3	1.5E-2	2.3E-2	5.1E-5	6.9E-5	3.7E-3	5.8E-4	6.3E-2	2.0E-2
MEP	kg N-eq	4.7E-8	5.9E-4	2.5E-4	4.6E-4	6.1E-6	6.8E-6	3.3E-5	4.3E-5	9.5E-4	1.7E-3
MDP	kg Fe-eq	3.6E-7	8.2E-3	1.6E-1	2.2E-1	2.9E-4	4.9E-4	7.2E-2	4.5E-3	6.3E-1	1.6E-2
ODP _{inf}	kg CFC-11-eq	2.8E-12	5.8E-8	4.3E-6	5.9E-6	4.4E-10	3.5E-9	2.6E-9	1.8E-8	3.4E-8	7.2E-8
PMFP	kg PM ₁₀ -eq	1.6E-7	7.4E-4	3.2E-3	4.6E-3	6.4E-6	1.6E-5	2.1E-4	8.6E-5	1.3E-2	1.9E-3
POFP	kg NMVOC	3.9E-7	1.3E-3	1.9E-3	2.9E-3	1.3E-5	4.9E-5	1.5E-4	2.0E-4	7.4E-3	3.1E-3
TAP ₁₀₀	kg SO ₂ -eq	5.1E-7	2.3E-3	1.4E-2	1.9E-2	1.9E-5	4.7E-5	2.2E-4	2.5E-4	5.6E-2	6.1E-3
TETP _{inf}	kg 1,4-DCB-eq	2.3E-9	5.4E-5	2.6E-4	2.2E-4	4.8E-7	6.7E-7	1.0E-5	6.0E-6	5.1E-4	1.1E-4

Impact Categories: global warming (GWP), fossil depletion (FDP), freshwater ecotoxicity (FETP), freshwater eutrophication (FEP), human toxicity (HTP), marine ecotoxicity (METP), marine eutrophication (MEP), metal depletion (MDP), ozone depletion (ODP), particulate matter formation (PMFP), terrestrial acidification (TAP), terrestrial ecotoxicity (ETEP) potentials. *Abbreviations:* 1,4-DCB refers to 1,4-dichlorobenzene, CFC-11 to trichlorofluoromethane, PM₁₀ to “particulate matter less than 10 µm in diameter”, NMVOC to “non methane volatile organic carbon”. The suffixes “inf” and “100” refer to infinity and 100 years, respectively.

Table S28: NCM Li-ion life cycle impact for storing and delivering 50 MJ of electrical energy to a power-train, broken down amongst key components

		Battery Use	Battery & Components Manufacture	Positive Electrode Paste	Negative Electrode Paste	Electrolyte	Separator	Cell Container	Module & Battery Casing	BMS	Substrate of Negative Electrode	Substrate of Positive Electrode	Electricity Consumed by Battery
GWP ₁₀₀	kg CO ₂ -eq	1.2E-5	3.1E-1	3.9E-1	8.7E-2	1.2E-2	6.0E-3	9.6E-2	3.6E-2	1.6E-1	1.5E-2	1.7E-2	7.4E-1
FDP	kg oil-eq	4.2E-6	1.0E-1	2.9E-2	4.4E-3	8.4E-3	3.8E-3	2.5E-2	1.9E-2	4.2E-2	4.6E-3	4.4E-3	2.1E-1
FETP _{inf}	kg 1,4-DCB-eq	3.7E-8	2.9E-3	4.5E-3	6.4E-5	6.3E-5	3.3E-5	1.0E-3	2.7E-4	1.6E-2	1.6E-2	1.9E-4	1.0E-2
FEP	kg P-eq	2.1E-9	2.1E-4	1.4E-4	3.8E-6	3.2E-6	1.8E-6	4.4E-5	1.6E-5	8.1E-4	7.7E-4	8.0E-6	7.3E-4
HTP _{inf}	kg 1,4-DCB-eq	1.7E-6	1.4E-1	2.4E-1	8.6E-3	3.1E-3	1.6E-3	4.3E-2	1.5E-2	1.4E+0	1.8E+0	7.8E-3	4.8E-1
METP _{inf}	kg 1,4-DCB-eq	6.9E-8	3.0E-3	4.6E-3	7.0E-5	6.1E-5	2.9E-5	1.1E-3	2.8E-4	1.6E-2	2.0E-2	2.0E-4	1.0E-2
MEP	kg N-eq	2.3E-8	2.5E-4	6.2E-4	1.9E-4	5.4E-6	2.9E-6	5.6E-5	2.1E-5	3.2E-4	2.1E-4	1.0E-5	8.4E-4
MDP	kg Fe-eq	1.8E-7	3.0E-3	3.8E-1	4.7E-4	6.4E-4	2.1E-4	4.8E-3	2.2E-3	2.0E-1	2.5E-1	8.7E-4	8.0E-3
ODP _{inf}	kg CFC-11-eq	1.4E-12	2.4E-8	9.0E-6	2.3E-6	1.1E-9	1.5E-9	6.5E-9	8.7E-9	1.7E-8	1.2E-9	1.2E-9	3.6E-8
PMFP	kg PM10-eq	7.8E-8	3.1E-4	1.0E-3	1.4E-5	1.5E-5	6.8E-6	1.9E-4	4.3E-5	3.8E-4	6.6E-4	3.4E-5	9.7E-4
POFP	kg NMVOC	1.9E-7	5.5E-4	8.0E-4	2.6E-5	3.9E-5	2.1E-5	2.4E-4	9.9E-5	6.8E-4	4.2E-4	4.4E-5	1.5E-3
TAP ₁₀₀	kg SO ₂ -eq	2.5E-7	9.7E-4	4.3E-3	4.9E-5	4.4E-5	2.0E-5	3.9E-4	1.2E-4	1.1E-3	2.1E-3	7.1E-5	3.1E-3
TETP _{inf}	kg 1,4-DCB-eq	1.1E-9	2.3E-5	7.6E-5	1.1E-6	1.0E-6	2.9E-7	9.2E-6	3.0E-6	3.7E-5	9.9E-5	1.7E-6	5.6E-5

Impact Categories: global warming (GWP), fossil depletion (FDP), freshwater ecotoxicity (FETP), freshwater eutrophication (FEP), human toxicity (HTP), marine ecotoxicity (METP), marine eutrophication (MEP), metal depletion (MDP), ozone depletion (ODP), particulate matter formation (PMFP), terrestrial acidification (TAP), terrestrial ecotoxicity (ETEP) potentials. *Abbreviations:* 1,4-DCB refers to 1,4-dichlorobenzene, CFC-11 to trichlorofluoromethane, PM10 to “particulate matter less than 10 µm in diameter”, NMVOC to “non methane volatile organic carbon”. The suffixes “inf” and “100” refer to infinity and 100 years, respectively.

Table S29: LFP Li-ion life cycle impact for storing and delivering 50 MJ of electrical energy to a power-train, broken down amongst key components

		Battery Use	Battery & Components Manufacture	Positive Electrode Paste	Negative Electrode Paste	Electrolyte	Separator	Cell Container	Module & Battery Casing	BMS	Substrate of Negative Electrode	Substrate of Positive Electrode	Electricity Consumed by Battery
GWP ₁₀₀	kg CO ₂ -eq	7.8E-6	2.0E-1	2.5E-1	4.7E-2	7.8E-3	3.8E-3	6.1E-2	2.3E-2	1.0E-1	9.7E-3	1.1E-2	7.4E-1
FDP	kg oil-eq	2.7E-6	6.4E-2	1.7E-2	2.4E-3	5.3E-3	2.4E-3	1.6E-2	1.2E-2	2.7E-2	2.9E-3	2.8E-3	2.1E-1
FETP _{inf}	kg 1,4-DCB-eq	2.3E-8	1.9E-3	4.8E-4	3.5E-5	4.0E-5	2.1E-5	6.6E-4	1.7E-4	1.0E-2	9.9E-3	1.2E-4	1.0E-2
FEP	kg P-eq	1.4E-9	1.3E-4	1.2E-4	2.0E-6	2.0E-6	1.1E-6	2.8E-5	1.0E-5	5.1E-4	4.9E-4	5.0E-6	7.3E-4
HTP _{inf}	kg 1,4-DCB-eq	1.1E-6	8.7E-2	3.3E-2	4.7E-3	2.0E-3	9.9E-4	2.7E-2	9.3E-3	8.7E-1	1.1E+0	4.9E-3	4.8E-1
METP _{inf}	kg 1,4-DCB-eq	4.4E-8	1.9E-3	5.0E-4	3.8E-5	3.9E-5	1.9E-5	6.9E-4	1.8E-4	1.0E-2	1.3E-2	1.2E-4	1.0E-2
MEP	kg N-eq	1.5E-8	1.6E-4	3.7E-4	1.0E-4	3.5E-6	1.9E-6	3.6E-5	1.3E-5	2.0E-4	1.3E-4	6.5E-6	8.4E-4
MDP	kg Fe-eq	1.1E-7	1.9E-3	3.1E-3	2.5E-4	4.1E-4	1.3E-4	3.0E-3	1.4E-3	1.2E-1	1.6E-1	5.5E-4	8.0E-3
ODP _{inf}	kg CFC-11-eq	8.9E-13	1.6E-8	6.1E-6	1.2E-6	6.7E-10	9.4E-10	4.1E-9	5.6E-9	1.1E-8	7.8E-10	7.4E-10	3.6E-8
PMFP	kg PM10-eq	4.9E-8	2.0E-4	9.9E-5	7.6E-6	9.3E-6	4.3E-6	1.2E-4	2.7E-5	2.4E-4	4.2E-4	2.1E-5	9.7E-4
POFP	kg NMVOC	1.2E-7	3.5E-4	1.4E-4	1.4E-5	2.5E-5	1.3E-5	1.5E-4	6.3E-5	4.4E-4	2.7E-4	2.8E-5	1.5E-3
TAP ₁₀₀	kg SO ₂ -eq	1.6E-7	6.2E-4	3.4E-4	2.6E-5	2.8E-5	1.3E-5	2.5E-4	7.8E-5	7.0E-4	1.3E-3	4.5E-5	3.1E-3
TETP _{inf}	kg 1,4-DCB-eq	7.2E-10	1.4E-5	7.7E-6	6.2E-7	6.6E-7	1.8E-7	5.8E-6	1.9E-6	2.4E-5	6.3E-5	1.1E-6	5.6E-5

Impact Categories: global warming (GWP), fossil depletion (FDP), freshwater ecotoxicity (FETP), freshwater eutrophication (FEP), human toxicity (HTP), marine ecotoxicity (METP), marine eutrophication (MEP), metal depletion (MDP), ozone depletion (ODP), particulate matter formation (PMFP), terrestrial acidification (TAP), terrestrial ecotoxicity (ETEP) potentials. *Abbreviations:* 1,4-DCB refers to 1,4-dichlorobenzene, CFC-11 to trichlorofluoromethane, PM10 to “particulate matter less than 10 µm in diameter”, NMVOC to “non methane volatile organic carbon”. The suffixes “inf” and “100” refer to infinity and 100 years, respectively.

10 Structural Path Analysis

The main paper cites particularly interesting results from structural path analysis (SPA). We here present a broader selection of these, covering the most important paths for a few impact categories. Thus, some of the most important paths causing GWP for NiMH, NCM and LFP batteries are presented in SPA S1, 4, and 7, respectively. Important path for human toxicity in the life cycle of NiMH and NCM were respectively reported in SPA S3 and 5. The freshwater ecotoxicity of NiMH (SPA S2), the marine ecotoxicity of NCM (SPA S6) and the ozone depletion related to LFP life cycle (SPA S8) were also reported. The impact of each path are presented in absolute terms, and relative to the total life cycle impact. As these are “raw” results, we present them to the highest level of resolution possible, without regards to uncertainty or significant figures.

SPA S1: Most important paths for global warming potential impacts of NiMH life cycle

ABSOLUTE (kg CO₂-eq); RELATIVE (%) : SEQUENCE>

0.1927189315; 5.465956725: Battery Use_ NiMH> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix DE> electricity, lignite, at power plant> lignite, burned in power plant

0.1692806747, 4.801193299: Battery Use_ NiMH> Battery Assembly_ NiMH> heat, natural gas, at industrial furnace low-NOx >100kW> natural gas, burned in industrial furnace low-NOx >100kW

0.1361297714; 3.860956647: Battery Use_ NiMH> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix DE> electricity, hard coal, at power plant> hard coal, burned in power plant

0.1152944725; 3.270019153: Battery Use_ NiMH> Battery Assembly_ NiMH> Negative Electrode_ AB5_MH_ NiMH> tetrafluoroethylene, at plant

0.08783795666; 2.491288563: Battery Use_ NiMH> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix PL> electricity, hard coal, at power plant> hard coal, burned in power plant

0.08417692071; 2.387453077: Battery Use_ NiMH> Battery Assembly_ NiMH> Positive Electrode Material_ Ni_ NiMH> tetrafluoroethylene, at plant

0.07608270577; 2.157882332: Battery Use_ NiMH> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix IT> electricity, natural gas, at power plant> natural gas, burned in power plant

0.07583573873; 2.150877773: Battery Use_ NiMH> Battery Assembly_ NiMH> Negative Electrode_ AB5_MH_ NiMH> tetrafluoroethylene, at plant> chlorodifluoromethane, at plant

0.07044034951; 997851997: Battery Use_ NiMH> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix ES> electricity, hard coal, at power plant> hard coal, burned in power plant

0.0688529278; 1.952829029: Battery Use_ NiMH> Battery Assembly_ NiMH> Substrate_ Nickel Foam_ NiMH> nickel, 99.5%, at plant> heavy fuel oil, burned in industrial furnace 1MW, non-modulating

0.06715870651; 1.904776976: Battery Use_ NiMH> Battery Assembly_ NiMH> Substrate_ Nickel Foam_ NiMH> nickel, 99.5%, at plant> portland calcareous cement, at plant> clinker, at plant

0.06335045909; 1.79676623: Battery Use_ NiMH> Battery Assembly_ NiMH> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix DE> electricity, lignite, at power plant> lignite, burned in power plant

0.06194660234; 1.75694959: Battery Use_ NiMH> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix PL> electricity, lignite, at power plant> lignite, burned in power plant

SPA S2: Most important paths for freshwater ecotoxicity potential impacts of NIMH life cycle

ABSOLUTE (kg-DCB-eq); RELATIVE(%): SEQUENCE:

0.02775295402; 22.17769266 : Battery Use_ NiMH> Battery Assembly_ NiMH> Substrate_ Nickel Foam_ NiMH> nickel, 99.5%, at plant> disposal, sulfidic tailings, off-site

0.02743987885; 21.92751083: Battery Use_ NiMH> Battery Assembly_ NiMH> Substrate_ Nickel Foam_ NiMH> nickel, 99.5%, at plant> disposal, nickel smelter slag, 0% water, to residual material landfill

0.009212175665; 7.361551515: Battery Use_ NiMH> Battery Assembly_ NiMH> Negative Electrode_ AB5_MH_ NiMH> nickel, 99.5%, at plant> disposal, sulfidic tailings, off-site

0.009108255072; 7.278507419: Battery Use_ NiMH> Battery Assembly_ NiMH> Negative Electrode_ AB5_MH_ NiMH> nickel, 99.5%, at plant> disposal, nickel smelter slag, 0% water, to residual material landfill

0.006974318485; 5.573255079: Battery Use_ NiMH> Battery Assembly_ NiMH> Positive Electrode Material_ Ni_ NiMH> Ni(OH)₂> NiSO₄> disposal, sulfidic tailings, off-site

0.006895683582; 5.510417057: Battery Use_ NiMH> Battery Assembly_ NiMH> Positive Electrode Material_ Ni_ NiMH> Ni(OH)₂> NiSO₄> disposal, nickel smelter slag, 0% water, to residual material landfill

0.006039023145; 4.825850223: Battery Use_ NiMH> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix DE> electricity, lignite, at power plant> lignite, burned in power plant> lignite, at mine> disposal, spoil from lignite mining, in surface landfill

0.002996682198; 2.394681905: Battery Use_ NiMH> Battery Assembly_ NiMH> Cell Container_ Stainless_ NiMH> steel, electric, chromium steel 18/8, at plant> ferronickel, 25% Ni, at plant> disposal, nickel smelter slag, 0% water, to residual material landfill

0.002131734694; 1.703492784: Battery Use_ NiMH> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix GR> electricity, lignite, at power plant> lignite, burned in power plant> lignite, at mine> disposal, spoil from lignite mining, in surface landfill

0.002095323202; 1.674395957: Battery Use_ NiMH> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix PL> electricity, lignite, at power plant> lignite, burned in power plant> lignite, at mine> disposal, spoil from lignite mining, in surface landfill

0.001985144302; 1.586350779: Battery Use_ NiMH> Battery Assembly_ NiMH> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix DE> electricity, lignite, at power plant> lignite, burned in power plant> lignite, at mine> disposal, spoil from lignite mining, in surface landfill

0.001277178099; 1.020607152: Battery Use_ NiMH> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix CZ> electricity, lignite, at power plant> lignite, burned in power plant> lignite, at mine> disposal, spoil from lignite mining, in surface landfill

SPA S3: Most important paths for human toxicity potential impacts of NiMH life cycle

ABSOLUTE (kg-DCB-eq); RELATIVE (%): SEQUENCE: >

2.351571375; 42.08278383: Battery Use_ NiMH> Battery Assembly_ NiMH> Substrate_ Nickel Foam_ NiMH> nickel, 99.5%, at plant> disposal, sulfidic tailings, off-site

0.7805687491; 13.96874714: Battery Use_ NiMH> Battery Assembly_ NiMH> Negative Electrode_ AB5_MH_ NiMH> nickel, 99.5%, at plant> disposal, sulfidic tailings, off-site

0.5909499833; 10.57540531: Battery Use_ NiMH> Battery Assembly_ NiMH> Positive Electrode Material_ Ni_ NiMH> Ni(OH)₂> NiSO₄> disposal, sulfidic tailings, off-site

0.2653040915; 4.747776254: Battery Use_ NiMH> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix DE> electricity, lignite, at power plant> lignite, burned in power plant> lignite, at mine> disposal, spoil from lignite mining, in surface landfill

0.09365056613; 1.675933196: Battery Use_ NiMH> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix GR> electricity, lignite, at power plant> lignite, burned in power plant> lignite, at mine> disposal, spoil from lignite mining, in surface landfill

0.09205095016; 1.647307106: Battery Use_ NiMH> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix PL> electricity, lignite, at power plant> lignite, burned in power plant> lignite, at mine> disposal, spoil from lignite mining, in surface landfill

0.0875864839; 1.567412798: Battery Use_ NiMH> Battery Assembly_ NiMH> Positive Electrode Material_ Ni_ NiMH> Ni(OH)₂> NiSO₄

0.08721061221; 1.560686348: Battery Use_ NiMH> Battery Assembly_ NiMH> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix DE> electricity, lignite, at power plant> lignite, burned in power plant> lignite, at mine> disposal, spoil from lignite mining, in surface landfill

0.05610850745; 1.004095481: Battery Use_ NiMH> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix CZ> electricity, lignite, at power plant> lignite, burned in power plant> lignite, at mine> disposal, spoil from lignite mining, in surface landfill

0.05020284007; 0.8984100117: Battery Use_ NiMH> Battery Assembly_ NiMH> Substrate_ Nickel Foam_ NiMH> nickel, 99.5%, at plant

0.01666407768; 0.2982136908: Battery Use_ NiMH> Battery Assembly_ NiMH> Negative Electrode_ AB5_MH_ NiMH> nickel, 99.5%, at plant

SPA S4: Most important paths for global warming potential impacts of NCM life cycle

ABSOLUTE (kg CO₂-eq); RELATIVE (%): SEQUENCE: >

0.178606742; 9.549869574: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Positive Electrode Material_ NCM Li-Ion> tetrafluoroethylene, at plant

0.1174798231; 6.281492933: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Positive Electrode Material_ NCM Li-Ion> tetrafluoroethylene, at plant> chlorodifluoromethane, at plant

0.09635946573; 5.152214969: Battery Use_ NCM Li-Ion> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix DE> electricity, lignite, at power plant> lignite, burned in power plant

0.07130220942; 3.812436152: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> heat, natural gas, at industrial furnace low-NO_x >100kW> natural gas, burned in industrial furnace low-NO_x >100kW

0.0680648857; 3.639340674: Battery Use_ NCM Li-Ion> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix DE> electricity, hard coal, at power plant> hard coal, burned in power plant

0.04510096718; 2.411489898: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Negative Electrode Material_ Carbon_ Li-Ion> tetrafluoroethylene, at plant

0.04391897833; 2.348290496: Battery Use_ NCM Li-Ion> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix PL> electricity, hard coal, at power plant> hard coal, burned in power plant

0.03804135288; 2.034021529: Battery Use_ NCM Li-Ion> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix IT> electricity, natural gas, at power plant> natural gas, burned in power plant

0.03522017475; 1.883176813: Battery Use_ NCM Li-Ion> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix ES> electricity, hard coal, at power plant> hard coal, burned in power plant

0.03097330117; 1.656102021: Battery Use_ NCM Li-Ion> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix PL> electricity, lignite, at power plant> lignite, burned in power plant

0.0296654739; 1.586174202: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Negative Electrode Material_ Carbon_ Li-Ion> tetrafluoroethylene, at plant> chlorodifluoromethane, at plant

0.02668365842; 1.426740417: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix DE> electricity, lignite, at power plant> lignite, burned in power plant

0.02612728078; 1.39699163: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Cell Container_Al_ Li-Ion> aluminum, production mix, at plant> aluminum, primary, at plant> aluminum, primary, liquid, at plant

0.02536983969; 1.356492243: Battery Use_ NCM Li-Ion> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix CZ> electricity, lignite, at power plant> lignite, burned in power plant

0.02282757596; 1.220560717: Battery Use_ NCM Li-Ion> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix GR> electricity, lignite, at power plant> lignite, burned in power plant

0.02123285324; 1.135292973: Battery Use_ NCM Li-Ion> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix IT> electricity, hard coal, at power plant> hard coal, burned in power plant

SPA S5: Most important paths for human toxicity potential impacts of NCM life cycle

ABSOLUTE (kg-DCB-eq); RELATIVE (%): SEQUENCE

1.072748568; 26.13494926: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Substrate_ Negative Electrode_ Li-Ion> copper, primary, at refinery> copper concentrate, at beneficiation> disposal, sulfidic tailings, off-site

0.5076544453; 12.36778456: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Substrate_ Negative Electrode_ Li-Ion> copper, primary, at refinery

0.329930081; 8.03795613: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Battery Management System> integrated circuit, IC, logic type, at plant> gold, primary, at refinery> gold, at refinery> disposal, sulfidic tailings, off-site>

0.3233980639; 7.878819181: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Battery Management System> integrated circuit, IC, logic type, at plant> gold, primary, at refinery> gold, at refinery> disposal, sulfidic tailings, off-site>

0.1936968565; 4.718959939: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Battery Management System> copper, primary, at refinery> copper concentrate, at beneficiation> disposal, sulfidic tailings, off-site

0.187533565; 4.568806104: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Substrate_ Negative Electrode_ Li-Ion> copper, primary, at refinery> copper, SX-EW, at refinery> disposal, sulfidic tailings, off-site

0.1546332005; 3.767267533: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Positive Electrode Material_ NCM Li-Ion> Li[Ni0.4Co0.2Mn0.4]O2> Ni0.4Co0.2Mn0.4(OH)2> NiSO4> disposal, sulfidic tailings, off-site>

0.1326520458; 3.231749349: Battery Use_ NCM Li-Ion> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix DE> electricity, lignite, at power plant> lignite, burned in power plant> lignite, at mine> disposal, spoil from lignite mining, in surface landfill

0.1034575354; 2.520495034: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Battery Management System> integrated circuit, IC, logic type, at plant> gold, primary, at refinery> gold, from combined gold-silver production, at refinery> disposal, sulfidic tailings, off-site>

0.09166273738; 2.233143033: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Battery Management System> copper, primary, at refinery

0.08779066324; 2.138809222: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Battery Management System> integrated circuit, IC, logic type, at plant> gold, primary, at refinery> gold, from combined gold-silver production, at refinery> disposal, sulfidic tailings, off-site>

0.04682528307; 1.14078586: Battery Use_ NCM Li-Ion> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix GR> electricity, lignite, at power plant> lignite, burned in power plant> lignite, at mine> disposal, spoil from lignite mining, in surface landfill

0.04602547508; 1.121300454: Battery Use_ NCM Li-Ion> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix PL> electricity, lignite, at power plant> lignite, burned in power plant> lignite, at mine> disposal, spoil from lignite mining, in surface landfill

SPA S6: Most important paths for marine ecotoxicity potential impacts of NCM life cycle

ABSOLUTE (kg-DCB-eq); RELATIVE (%): SEQUENCE: >

0.0115998848; 20.87767762: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Substrate_ Negative Electrode_ Li-Ion> copper, primary, at refinery> copper concentrate, at beneficiation> disposal, sulfidic tailings, off-site

0.005406292186; 9.730340203: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Substrate_ Negative Electrode_ Li-Ion> copper, primary, at refinery

0.003567612249; 6.421051564: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Battery Management System> integrated circuit, IC, logic type, at plant> gold, primary, at refinery> gold, at refinery> disposal, sulfidic tailings, off-site>

0.003496979999; 6.293926392: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Battery Management System> integrated circuit, IC, logic type, at plant> gold, primary, at refinery> gold, at refinery> disposal, sulfidic tailings, off-site>

0.002908245692; 5.234311984: Battery Use_ NCM Li-Ion> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix DE> electricity, lignite, at power plant> lignite, burned in power plant> lignite, at mine> disposal, spoil from lignite mining, in surface landfill

0.002094490068; 3.769700233: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Battery Management System> copper, primary, at refinery> copper concentrate, at beneficiation> disposal, sulfidic tailings, off-site

0.002027844935; 3.649751144: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Substrate_ Negative Electrode_ Li-Ion> copper, primary, at refinery> copper, SX-EW, at refinery> disposal, sulfidic tailings, off-site

0.001762993191; 3.173066296: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Positive Electrode Material_ NCM Li-Ion> Li[Ni0.4Co0.2Mn0.4]O2> Ni0.4Co0.2Mn0.4(OH)2> NiSO4> disposal, nickel smelter slag, 0% water, to residual material landfill>

0.001672085488; 3.009449005: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Positive Electrode Material_ NCM Li-Ion> Li[Ni0.4Co0.2Mn0.4]O2> Ni0.4Co0.2Mn0.4(OH)2> NiSO4> disposal, sulfidic tailings, off-site>

0.00118710878; 2.013475604: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Battery Management System> integrated circuit, IC, logic type, at plant> gold, primary, at refinery> gold, from combined gold-silver production, at refinery> disposal, sulfidic tailings, off-site>

0.001026591237; 1.847677048: Battery Use_ NCM Li-Ion> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix GR> electricity, lignite, at power plant> lignite, burned in power plant> lignite, at mine> disposal, spoil from lignite mining, in surface landfill

0.001009056354; 1.816117455: Battery Use_ NCM Li-Ion> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix PL> electricity, lignite, at power plant> lignite, burned in power plant> lignite, at mine> disposal, spoil from lignite mining, in surface landfill

0.0009761670471; 1.7569227: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Battery Management System> copper, primary, at refinery

0.000949301272; 1.708569203: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> Battery Management System> integrated circuit, IC, logic type, at plant> gold, primary, at refinery> gold, from combined gold-silver production, at refinery> disposal, sulfidic tailings, off-site>

0.000805345215; 1.449474548: Battery Use_ NCM Li-Ion> Battery Assembly_ NCM Li-Ion> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix DE> electricity, lignite, at power plant> lignite, burned in power plant> lignite, at mine> disposal, spoil from lignite mining, in surface landfill

0.0006150577028; 1.106991721: Battery Use_ NCM Li-Ion> Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix CZ> electricity, lignite, at power plant> lignite, burned in power plant> lignite, at mine> disposal, spoil from lignite mining, in surface landfill

SPA S7: Most important paths for global warming potential impacts of LFP life cycle

ABSOLUTE (kg CO₂-eq); RELATIVE (%): SEQUENCE

0.1214788503; 8.37916902: Battery Use_ LFP Li-Ion > Battery Assembly_ LFP Li-Ion> Positive Electrode Material_ LFP Li-Ion> tetrafluoroethylene, at plant

0.09635946573; 6.646525285: Battery Use_ LFP Li-Ion > Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix DE> electricity, lignite, at power plant> lignite, burned in power plant

0.07990355613; 5.511456526: Battery Use_ LFP Li-Ion > Battery Assembly_ LFP Li-Ion> Positive Electrode Material_ LFP Li-Ion> tetrafluoroethylene, at plant> chlorodifluoromethane, at plant>

0.0680648857; 4.694868121: Battery Use_ LFP Li-Ion > Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix DE> electricity, hard coal, at power plant> hard coal, burned in power plant

0.04542624037; 3.13333675: Battery Use_ LFP Li-Ion > Battery Assembly_ LFP Li-Ion> heat, natural gas, at industrial furnace low-NO_x >100kW> natural gas, burned in industrial furnace low-NO_x >100kW

0.04391897833; 3.0293713: Battery Use_ LFP Li-Ion > Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix PL> electricity, hard coal, at power plant> hard coal, burned in power plant

0.03804135288; 2.623954086: Battery Use_ LFP Li-Ion > Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix IT> electricity, natural gas, at power plant> natural gas, burned in power plant

0.03522017475; 2.429359485: Battery Use_ LFP Li-Ion > Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix ES> electricity, hard coal, at power plant> hard coal, burned in power plant

0.03097330117; 2.1364256: Battery Use_ LFP Li-Ion > Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix PL> electricity, lignite, at power plant> lignite, burned in power plant

0.02536983969; 1.749919219: Battery Use_ LFP Li-Ion > Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix CZ> electricity, lignite, at power plant> lignite, burned in power plant

0.02454023214; 1.692695909: Battery Use_ LFP Li-Ion > Battery Assembly_ LFP Li-Ion> Negative Electrode Material_ Carbon_ Li-Ion> tetrafluoroethylene, at plant

0.02282757596; 1.574563118: Battery Use_ LFP Li-Ion > Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix GR> electricity, lignite, at power plant> lignite, burned in power plant

0.02123285324; 1.464564948: Battery Use_ LFP Li-Ion > Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix IT> electricity, hard coal, at power plant> hard coal, burned in power plant

0.01909755904; 1.317280125: Battery Use_ LFP Li-Ion > Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix IT> electricity, oil, at power plant> heavy fuel oil, burned in power plant

0.01817547635; 1.253678216: Battery Use_ LFP Li-Ion > Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix NL> electricity, natural gas, at power plant> natural gas, burned in power plant

0.0175330133; 1.209363453: Battery Use_ LFP Li-Ion > Electricity Consumed by Battery> electricity, medium voltage, production UCTE, at grid> electricity, high voltage, production UCTE, at grid> electricity, production mix UCTE> electricity, production mix CS> electricity, lignite, at power plant> lignite, burned in power plant

SPA S8: Most important paths for ozone depletion potential impacts of LFP life cycle

ABSOLUTE (kg CFC-11-eq); RELATIVE (%): SEQUENCE

3.555761239e-06; 47.62642565: Battery Use_ LFP Li-Ion > Battery Assembly_ LFP Li-Ion> Positive Electrode Material_ LFP Li-Ion> tetrafluoroethylene, at plant

1.379044274e-06; 18.47113605: Battery Use_ LFP Li-Ion > Battery Assembly_ LFP Li-Ion> Positive Electrode Material_ LFP Li-Ion> tetrafluoroethylene, at plant> chlorodifluoromethane, at plant> trichloromethane, at plant

1.206073396e-06; 16.15433688: Battery Use_ LFP Li-Ion > Battery Assembly_ LFP Li-Ion> Positive Electrode Material_ LFP Li-Ion> tetrafluoroethylene, at plant> chlorodifluoromethane, at plant

7.183078044e-07; 9.621127783: Battery Use_ LFP Li-Ion > Battery Assembly_ LFP Li-Ion> Negative Electrode Material_ Carbon_ Li-Ion> tetrafluoroethylene, at plant

2.785840213e-07; 3.731398227: Battery Use_ LFP Li-Ion > Battery Assembly_ LFP Li-Ion> Negative Electrode Material_ Carbon_ Li-Ion> tetrafluoroethylene, at plant> chlorodifluoromethane, at plant> trichloromethane, at plant

2.436417618e-07; 3.263376103: Battery Use_ LFP Li-Ion > Battery Assembly_ LFP Li-Ion> Negative Electrode Material_ Carbon_ Li-Ion> tetrafluoroethylene, at plant> chlorodifluoromethane, at plant

11 Sensitivity Analysis

In order to have a better grasp on the confidence intervals associated with our main results, a sensitivity analysis was performed. Selected battery characteristics and production parameters were altered, and the impacts of these alterations on the final mid-point indicator results was assessed (Table S30). For this analysis, we selected parameters we deemed would have the strongest impact, and the relative alterations strive to be representative of the inhomogeneity of the system.

Table S30: Sensitivity Analysis

FU: Charge-discharge 50 MJ		Control			Chinese Electricity Mix		
		NCM	LFP	NIMH	NCM	LFP	NIMH
climate change	kg CO ₂ -eq	1.9E+0	1.4E+0	3.5E+0	2.1E+0	1.6E+0	4.1E+0
fossil depletion	kg oil-eq	4.5E-1	3.7E-1	9.9E-1	4.9E-1	3.9E-1	1.1E+0
freshwater ecotoxicity	kg 1,4-DCB-eq	5.1E-2	3.4E-2	1.3E-1	5.0E-2	3.3E-2	1.2E-1
freshwater eutrophication	kg P-eq	2.7E-3	2.0E-3	4.5E-3	2.6E-3	1.9E-3	4.2E-3
human toxicity	kg 1,4-DCB-eq	4.1E+0	2.7E+0	5.6E+0	4.0E+0	2.6E+0	5.4E+0
marine ecotoxicity	kg 1,4-DCB-eq	5.6E-2	3.7E-2	1.3E-1	5.4E-2	3.6E-2	1.3E-1
marine eutrophication	kg N-eq	2.5E-3	1.9E-3	4.0E-3	2.5E-3	1.9E-3	4.0E-3
metal depletion	kg Fe-eq	8.5E-1	3.0E-1	1.1E+0	8.5E-1	3.0E-1	1.1E+0
ozone depletion	kg CFC-11-eq	1.1E-5	7.5E-6	1.0E-5	1.1E-5	7.5E-6	1.0E-5
particulate matter formation	kg PM10-eq	3.6E-3	2.1E-3	2.3E-2	4.6E-3	2.7E-3	2.6E-2
photochemical oxidant formation	kg NMVOC	4.5E-3	3.0E-3	1.7E-2	5.8E-3	3.8E-3	2.0E-2
terrestrial acidification	kg SO ₂ -eq	1.2E-2	6.5E-3	9.8E-2	1.5E-2	8.4E-3	1.1E-1
terrestrial ecotoxicity	kg 1,4-DCB-eq	3.1E-4	1.7E-4	1.2E-3	3.0E-4	1.7E-4	1.2E-3
		-5% Efficiency			+5% Efficiency		
		NCM	LFP	NIMH	NCM	LFP	NIMH
climate change	kg CO ₂ -eq	2.2E+0	1.8E+0	3.8E+0	1.5E+0	1.1E+0	3.2E+0
fossil depletion	kg oil-eq	5.5E-1	4.6E-1	1.1E+0	3.6E-1	2.7E-1	9.0E-1
freshwater ecotoxicity	kg 1,4-DCB-eq	5.6E-2	3.8E-2	1.3E-1	4.7E-2	2.9E-2	1.2E-1
freshwater eutrophication	kg P-eq	3.0E-3	2.4E-3	4.8E-3	2.4E-3	1.7E-3	4.3E-3
human toxicity	kg 1,4-DCB-eq	4.3E+0	2.9E+0	5.8E+0	3.9E+0	2.4E+0	5.4E+0
marine ecotoxicity	kg 1,4-DCB-eq	6.0E-2	4.1E-2	1.4E-1	5.1E-2	3.2E-2	1.3E-1
marine eutrophication	kg N-eq	2.9E-3	2.2E-3	4.4E-3	2.1E-3	1.5E-3	3.7E-3
metal depletion	kg Fe-eq	8.5E-1	3.1E-1	1.1E+0	8.4E-1	3.0E-1	1.1E+0
ozone depletion	kg CFC-11-eq	1.1E-5	7.5E-6	1.0E-5	1.1E-5	7.4E-6	1.0E-5
particulate matter formation	kg PM10-eq	4.1E-3	2.5E-3	2.4E-2	3.2E-3	1.7E-3	2.3E-2
photochemical oxidant formation	kg NMVOC	5.2E-3	3.7E-3	1.8E-2	3.8E-3	2.3E-3	1.6E-2
terrestrial acidification	kg SO ₂ -eq	1.4E-2	7.9E-3	9.9E-2	1.1E-2	5.1E-3	9.7E-2
terrestrial ecotoxicity	kg 1,4-DCB-eq	3.3E-4	2.0E-4	1.2E-3	2.8E-4	1.5E-4	1.2E-3
		-25% Density			+25% Density		
		NCM	LFP	NIMH	NCM	LFP	NIMH
climate change	kg CO ₂ -eq	2.0E+0	1.5E+0	3.9E+0	1.8E+0	1.4E+0	3.3E+0
fossil depletion	kg oil-eq	4.9E-1	3.9E-1	1.1E+0	4.3E-1	3.5E-1	9.3E-1
freshwater ecotoxicity	kg 1,4-DCB-eq	6.7E-2	4.4E-2	1.7E-1	4.2E-2	2.8E-2	1.0E-1
freshwater eutrophication	kg P-eq	3.5E-3	2.5E-3	5.6E-3	2.3E-3	1.7E-3	3.9E-3
human toxicity	kg 1,4-DCB-eq	5.7E+0	3.7E+0	7.3E+0	3.1E+0	2.0E+0	4.5E+0
marine ecotoxicity	kg 1,4-DCB-eq	7.4E-2	4.8E-2	1.8E-1	4.4E-2	2.9E-2	1.1E-1
marine eutrophication	kg N-eq	2.8E-3	2.0E-3	4.7E-3	2.4E-3	1.8E-3	3.6E-3
metal depletion	kg Fe-eq	1.1E+0	4.5E-1	1.6E+0	7.1E-1	2.2E-1	8.3E-1
ozone depletion	kg CFC-11-eq	1.1E-5	7.5E-6	1.0E-5	1.1E-5	7.5E-6	1.0E-5
particulate matter formation	kg PM10-eq	4.3E-3	2.5E-3	3.2E-2	3.2E-3	1.8E-3	1.8E-2
photochemical oxidant formation	kg NMVOC	5.2E-3	3.5E-3	2.2E-2	4.1E-3	2.8E-3	1.4E-2
terrestrial acidification	kg SO ₂ -eq	1.4E-2	7.7E-3	1.4E-1	1.1E-2	5.7E-3	7.6E-2
terrestrial ecotoxicity	kg 1,4-DCB-eq	3.9E-4	2.3E-4	1.5E-3	2.6E-4	1.4E-4	9.7E-4

Table S30: Sensitivity Analysis (cont'd)

		-33% lifetime			+33% lifetime		
		NCM	LFP	NIMH	NCM	LFP	NIMH
climate change	kg CO ₂ -eq	2.4E+0	1.8E+0	4.6E+0	1.6E+0	1.3E+0	3.0E+0
fossil depletion	kg oil-eq	5.8E-1	4.4E-1	1.3E+0	3.9E-1	3.3E-1	8.5E-1
freshwater ecotoxicity	kg 1,4-DCB-eq	7.2E-2	4.6E-2	1.8E-1	4.1E-2	2.8E-2	9.9E-2
freshwater eutrophication	kg P-eq	3.7E-3	2.7E-3	6.1E-3	2.2E-3	1.7E-3	3.8E-3
human toxicity	kg 1,4-DCB-eq	5.9E+0	3.8E+0	7.9E+0	3.2E+0	2.1E+0	4.4E+0
marine ecotoxicity	kg 1,4-DCB-eq	7.8E-2	5.0E-2	1.9E-1	4.4E-2	3.0E-2	1.1E-1
marine eutrophication	kg N-eq	3.4E-3	2.4E-3	5.2E-3	2.1E-3	1.6E-3	3.4E-3
metal depletion	kg Fe-eq	1.3E+0	4.5E-1	1.7E+0	6.4E-1	2.3E-1	8.4E-1
ozone depletion	kg CFC-11-eq	1.7E-5	1.1E-5	1.5E-5	8.6E-6	5.6E-6	7.8E-6
particulate matter formation	kg PM10-eq	5.0E-3	2.7E-3	3.4E-2	3.0E-3	1.8E-3	1.8E-2
photochemical oxidant formation	kg NMVOC	5.9E-3	3.8E-3	2.4E-2	3.7E-3	2.7E-3	1.4E-2
terrestrial acidification	kg SO ₂ -eq	1.7E-2	8.2E-3	1.4E-1	9.9E-3	5.6E-3	7.5E-2
terrestrial ecotoxicity	kg 1,4-DCB-eq	4.3E-4	2.3E-4	1.7E-3	2.4E-4	1.5E-4	9.1E-4
		-33% Manufacture Energy			+33% Manufacture Energy		
		NCM	LFP	NIMH	NCM	LFP	NIMH
climate change	kg CO ₂ -eq	1.8E+0	1.4E+0	3.3E+0	2.0E+0	1.5E+0	3.8E+0
fossil depletion	kg oil-eq	4.2E-1	3.4E-1	9.1E-1	4.9E-1	3.9E-1	1.1E+0
freshwater ecotoxicity	kg 1,4-DCB-eq	5.0E-2	3.3E-2	1.2E-1	5.2E-2	3.4E-2	1.3E-1
freshwater eutrophication	kg P-eq	2.7E-3	2.0E-3	4.4E-3	2.8E-3	2.1E-3	4.7E-3
human toxicity	kg 1,4-DCB-eq	4.1E+0	2.6E+0	5.5E+0	4.2E+0	2.7E+0	5.7E+0
marine ecotoxicity	kg 1,4-DCB-eq	5.5E-2	3.6E-2	1.3E-1	5.7E-2	3.7E-2	1.4E-1
marine eutrophication	kg N-eq	2.4E-3	1.8E-3	3.8E-3	2.6E-3	1.9E-3	4.2E-3
metal depletion	kg Fe-eq	8.5E-1	3.0E-1	1.1E+0	8.5E-1	3.1E-1	1.1E+0
ozone depletion	kg CFC-11-eq	1.1E-5	7.5E-6	1.0E-5	1.1E-5	7.5E-6	1.0E-5
particulate matter formation	kg PM10-eq	3.5E-3	2.0E-3	2.3E-2	3.7E-3	2.2E-3	2.4E-2
photochemical oxidant formation	kg NMVOC	4.3E-3	2.9E-3	1.7E-2	4.7E-3	3.2E-3	1.7E-2
terrestrial acidification	kg SO ₂ -eq	1.2E-2	6.3E-3	9.7E-2	1.2E-2	6.7E-3	9.9E-2
terrestrial ecotoxicity	kg 1,4-DCB-eq	3.0E-4	1.7E-4	1.2E-3	3.1E-4	1.8E-4	1.2E-3

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