

SUPPORTING INFORMATION FOR:

Degen, F., Mitterfellner, M. & Kampker, A. (2024) Comparative life cycle assessment of lithium-ion, sodium-ion and solid-state battery cells for electric vehicles. *Journal of Industrial Ecology.*



This supporting information provides information about the made assumptions, about the used information sources as well as about the used formulae for calculation.



**Design and recipes of today's battery cell chemistries**

First, we analysed which battery cells are currently being installed in electric vehicles. We used the Fraunhofer ISI Battery database, in which 1100 xEV models between 2010 and 2023 and more than 500 other models announced for 2023-2027 are listed. Parts of the database are available online (Fraunhofer Institute for Systems and Innovation Research ISI 2023). A meta-analysis of cell design over the last 10 years to date is provided by Link et. al, in particular with regard to coating thickness of the cathode, coating thickness of the anode, thickness of the aluminium foil, thickness of the copper foil, thickness of the separator, porosity of the anode, porosity of the cathode (Link, Neef, and Wicke 2023). Based on this data from battery cells in EVs, we worked with a team of cell designers in several workshops to derive electrode stacks as they are currently installed in EVs. First, a variable parameter was defined, from which the rest of the variable cell parameters can be calculated. We defined the calendared layer thickness of the cathode (tc,i,j) as the variable parameter, with i for the respective cell chemistry (NCA, NMC532, NMC622, NMC811, NMC900, LFP) and j for the cell configuration (HE, HP). This was defined for all cell chemistries with tc,i,HP=50 µm for high power configurations and with tc,i,HE=90 µm for high energy configurations. From this, in combination with the pore share (φ), the weight share (w) and the density (ρ) of active material, binder and carbon black the mass per area of the cathode (mA,c) can be calculated:

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From this, in combination with the specific capacity of the cathode active material (Cg,CAM), the areal capacity for a cathode coated on one side (CA,c) can be calculated:

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This was then used to calculate the required area capacity of the anode (CA,a), assuming that this has a 10% higher capacity than the cathode:

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From this, the required anode active material mass per area (mA,AAM) can be calculated:

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From this, in combination with the weight share (w), the mass per area of the binder and carbon black can be calculated:

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The thickness of the anode can then be calculated in combination with the pore share of anode:

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The areal energy of a double-sided coated anode and cathode stack results from the cell voltage (U):

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**Material flows along the value-chain**

The material flow is analysed starting from the production of the precursor. The reason for this is that the material extraction production processes before precursor production can vary greatly. We assume that the production of the NCA and NMC precursor is hydrothermal (Dunn et al. 2015; Dai et al. 2018):

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In addition to the material, this requires an energy input of 11.32 kWh of natural gas per kg of precoursor (Dai et al. 2018). The reaction takes place in water, which is subsequently reprocessed and reused. However, 0.64 liters of water are lost per kg of precursor (Dai et al. 2018).

We assume that all analysed cathode active materials are produced by solid-state synthesis (Dai et al. 2018; Dunn et al. 2015). The lithium source is either Li2CO3 (for NMC532, NMC622, LFP):

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Or LiOH (for NCA, NMC811, NMC900):

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For the solid-state synthesis of NMC532 and NMC622, 6.35 kWh of electricity are necessary for per kg of active material (Dai et al. 2018). We assume the same amount for the solid-state synthesis of LFP. For the solid-state synthesis of NMC811 and NCA, 7.26 kWh of electricity are necessary for per kg of active material (Dai et al. 2018). We assume the same amount for the solid-state synthesis of NMC900.

The required mass and molar quantity of the raw materials can be calculated from the stoichiometry and the respective atomic mass. This results in the mass mE required to produce Ecell = 1 kWhcell of cell energy. The waste materials or by-products also result from the stoichiometry. A stoichiometric assumption is allowed as the material efficiency of synthesis factories is almost 100% (Dai et al. 2018).

For the subsequent battery cell production, we used the model of an industrial LIB production line (Degen and Krätzig 2023; Degen and Schütte 2022). This line produces 200 round cells (21700 format) per minute. This corresponds to the processing of 840m² of electrode stacks per hour and approximately 1 GWhcell/a of production capacity. Gigafactories that are being built today consist of several such production lines (Degen et al. 2023).

**Environmental impact of the input materials and of the complete battery cell**

The environmental damage potentials of the raw materials (e.g. NiSO4, CoSO4, MnSO4, AlSO4, LiOH, Li2CO3 etc.) were determined according to ReCiPe2016 v1.1 (H), taken from the Ecoinvent v3.8 database and calculated using GaBi 10.6.1.35.

The data taken from this has a log-normal distribution. This is defined in Ecoinvent by the median µ\* and the standard deviation σ\*. The standard deviation is obtained by an algorithm, based on basic uncertainty and by values obtained by a pedigree matrix. The standard deviations can be between σ\*=1.025 (for a pedigree matrix of [1,1,1,1,1]) and σ\*=1.582 (for a pedigree matrix of [5,5,5,5,5]) for resource flows. For materials where no σ\* is given, we assume σ\*=1.36 as default for a pedigree matrix of [3,5,5,5,4]. The 67% confidence interval can be calculated with the lower bound (LB\*) and the upper bound (UB\*) (Ciroth 2012):

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The median (µ\*), of an impact category (IC), for a certain battery component (bc), to achieve 1kWhcell of cell energy (E), is calculated as followed.

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σ\* respectively σbc\* for a certain battery component is unchanged by this multiplication, as the log-normal distribution is used. However, the median (µ\*), of an impact category (IC), for the entire stack, to achieve 1 kWhcell of cell energy (E) is calculated by:

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To be able to sum up also the standard deviation the log-normal distribution is transferred to the normal distribution, with:

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With this the variance VAR is calculated:

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And also the mean M is calculated:

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The variances of an impact category (IC), for a certain battery component (bc), to achieve 1kWhcell of cell energy (E), can be summed up:

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The 67% confidence interval can be approximated with the lower bound (LB) and the upper bound (UB):

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This is done for each cell chemistry (i) for each cell configuration (j).

Additional assumptions

As the damage potentials for electrolyte and anode binder (CMC-SBR) are not included, these were calculated as follows:

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During precursor production, material synthesis and cell production, energy is used in addition to the material, namely in the form of natural gas and/or electricity. Here we have used the following values for PED and GWP (values for other impact categories can be found in the attached calculation table):

Electricity: 1 kWhelectricity= 3.1 kWhPED and 1 kWhelectricity= 0.384 kgCO2-eq

Natural gas: 1 kWhnatural gas= 1 kWhPED and 1 kWhnatural gas= 0.186 kgCO2-eq

In cases where CO2 is generated during material synthesis (e.g. when synthesising with Li2CO3), this was added to the GWP.

**Sensitivity analysis and optimization potential**

We have calculated how various trends in battery cell design and battery production affect the environmental impact of battery cells. We analysed the following: Reconditioning of NMP; reduction of copper and aluminium foil thickness; optimisation of production technology in LIB gigafactories; use of electricity instead of natural gas; use of water as a solvent instead of NMP; larger casings, with thinner walls, made of aluminum; coating of active material; dry coating of anode.

Reconditioning of NMP

We have assumed that almost 100% of the NMP used as a solvent in electrode production can be recovered. This is also required by most emission laws in many countries. In the EU, NMP is classified as a "substance of very high concern" and is subject to strict regulations. NMP is either disposed of by incineration or reconditioned. Many gigafactories that are currently being built have their own internal reconditioning of NMP. There the NMP is distilled three times (n=3) by means of vacuum distillation at approx. Tp=125°C. Around λ=90% of the NMP can then be reused. The theoretically required energy input is calculated as follows:

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With Tr=25°C, cp=2.0 J/gK, M=10.09 mol/kg and ΔHvap=37kJ/mol.

This results in:

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We assume, analogous to the assumptions of Dunn et al.(Dunn et al. 2015) (engineering approach) to Dai et al.(Dai et al. 2018) (factory assessment) in NMC synthesis, the actual energy requirement is approx. 4 times higher than the theoretically derived value. This results in an approximate energy requirement of

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Reduction of current collector foil thickness

We have assumed a copper foil thickness of 10 µm in our basic scenario. This is produced by rolling. However, the current goal is to further reduce the thickness of the copper foil, to increase the gravimetric energy density of the LIB cells(Link, Neef, and Wicke 2023). Electrodepositing makes it possible to produce copper foils with a thickness of just a few µm. However, the reduced tensile strength and tear resistance are problematic with these low foil thicknesses. This can lead to tearing of the foils in the LIB factory and thus to long downtimes. However, it is currently assumed that with increasing process knowledge and thus process stability, thicknesses of 6 µm are realistic and achievable in the medium term. We assume a reduction in damage potential of 40% per m² of copper foil in in accordance with the change in thickness.

The same development trend exists, and the same challenges exist for the aluminium foil. In our basic scenario, we have assumed a aluminium foil thickness of 15 µm. An aluminium foil thickness of 10 µm is realistic in the medium term. We assume a reduction in the damage potential of 33% per m² of aluminium foil in accordance with the change in thickness.

LIB factory: optimized production technology

Degen et al. have shown that energy savings of 52.1% are possible in the gigafactories due to new production technologies (Degen et al. 2023). However, these numbers are partly based on advanced production technologies such as dry coating, which will probably not reach series production maturity on the cathode side for several years. We have therefore adopted technological improvements that are already being tested in the gigafactories, namely near-infrared drying, macro-environments and high c-rate formation. By consistently utilising these three technological approaches, an energy reduction of about 25% is possible in the LIB Gigafactory (Degen et al. 2023).

LIB factory: electricity instead of natural gas

More and more battery factories are being built in Europe that do not use natural gas and instead use electricity as an energy source. One reason for this is the increased cost of natural gas as a result of the conflict between Russia and Ukraine. Another reason is that electricity can be sourced CO2-neutrally, but natural gas cannot. Therefore, LIB Gigafactories are theoretically able to produce CO2-neutral in the future if the economic or political situation requires it. We assume that heat pumps are used to generate heat using electricity. We assume a coefficient of performance (COP), i.e. a conversion rate from electricity to heat of 2 for high temperature heat pumps(Degen et al. 2023; Arpagaus et al. 2018).

Water as solvent instead of NMP

While water is already used as a solvent for the binder in the production of the graphite anode, the use of water on the cathode side is challenging as the active material on the cathode side, the lithium oxide, can react with the water. This is particularly the case in cathode materials with a high nickel content. Thus, LiFePO4 is less reactive towards water and a reaction can be prevented with appropriate coatings. In most cases, carbon is applied to the LiFePO4 particles in a layer a few nanometres thick. This is usually done by adding carbon between the calcination steps. As we are dealing with the addition of only very small quantities of a widely available material (carbon) to an existing process (calcination), we have neglected the changes in the material input and only considered the change from NMP to water as a solvent.

Larger casings, with thinner walls, made of aluminum

There is a trend towards larger and lighter cell formats in battery cells for electric vehicles. The main aim here is to reduce the share of the case weight in the overall pack and thus increase the gravimetric energy density of the battery pack(Link, Neef, and Wicke 2023). While Tesla uses cylindrical 4680 casings made of steel, BYD uses aluminium casings with a wall thickness of 0.3 mm in its prismatic blade cells. BMW uses 46120 casings, which are 50% larger than those of Tesla. In our study, we adopt the BMW format (cylindrical cell, 46 mm diameter, 120 mm height), as well as the material choice (aluminium) and wall thickness (0.3 mm) of BYD.

Coating of cathode active material

The cathode active material can be coated to improve selected properties of this. For example, LFP can be coated with carbon. NCA and NMC can be coated with e.g. Al2O3 or ZrO. In LFP coating, the final active material is usually coated by fluidised bed coating right after material synthesis. In our study, we assume a weight proportion of 2% of the carbon coating. Here, we assume carbon black as the carbon source. Furthermore, we assume an energy input of 1 kWh/kg for fluidised bed coating. The coating of NCA and NMC usually takes place during material synthesis, usually by adding the coating additives before the final calcination step (Dai et al. 2018). In our study, we assume that ZrO is coated. Here, too, we assume a weight proportion of 2% of the ZrO coating.

Modified anode material mix for dry coating

Tear downs of battery cells from Tesla show that Tesla is already using dry coating on the anode side (Taylor 2022). The tear downs also show that the anode material mix had to be modified for this. For example, Tesla has completely avoided adding SiO to the graphite (Taylor 2022). In addition, the percentage of binder material in the mix is increased. Furthermore, PVDF is used as a binder instead of CMC-SBR. In our study we assume a mixing ratio of graphite/PVDF binder/carbon black of 95%/4%/1%. We also assume that the energy for drying the anode is eliminated, as is the material flow for the previous solvent (water) and for the previously used binder (CMC-SBR). However, the energy required for the mixing and application process for dry coating is higher than for the conventional process route (Degen et al. 2023).

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