

Supporting information 1:

Comparative sustainability assessment of lithium-ion, lithium-sulfur, and all-solid-state traction batteries

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S1-1: Detailed description of the system boundaries and assumptions made

The system boundaries include three different systems: the foreground system, the intermediate system, and the background system. A detailed description of the three systems and the assumptions made within them are provided in the following subsections.

S1-1.1 Foreground system

S1-1.1.1 Structure and composition of the battery systems

The foreground system includes the unit processes created to assess the ten batteries. The Battery Performance and Cost model 4.0 (BatPaC) (Nelson et al., 2019) is used to determine the composition of the batteries, which is referred to as "own calculation" in the tables in Supporting Information 2. For the lithium-ion battery calculation, the default BatPaC datasets are used. To represent the future battery types, the BatPaC is adapted to calculate the composition of LSBs and ASSBs. Therefore, a new dataset is created in the "Chem" spreadsheet for each of the six battery types. These new datasets differ from the datasets for lithium-ion batteries in several ways. First, no entry is required for the liquid electrolyte, so this

section is deleted. Instead, the section for the separator is expanded to include a representation of the solid electrolyte. In addition to the Information on the separator thickness and density, Information on the proportion of solid electrolyte material and binder with the respective density is added. The solid electrolyte material has a proportion of 97.44%, and the binder has a proportion of 2.56% (Schnell et al., 2020). Moreover, the section of the anode is modified to represent the use of lithium metal as a negative active material. For this, the data described by Deng et al. are used (Deng et al., 2017). Furthermore, two additional lines are added to the cathode section describing the proportion and density of the solid electrolyte material used in the positive electrode paste. The composition of the positive electrode paste for the ASSB-NCA, ASSB-LFP, ASSB-NMC622, and ASSB-NMC811 is divided into the following proportions: positive active material 78.99%, binder 1.40%, conductive additive 2.80%, and solid electrolyte material 16.81% (Randau et al., 2020; Schnell et al., 2020). Based on these definitions and extensions, the formulas in the BatPaC spreadsheets are adjusted. Besides, the parts not needed for the batteries, such as the cooling system, are deleted. Table 1 represents the key parameters defined for each investigated battery.

Table 1 - Key parameters of the investigated batteries

Component		LIB-NCA	LIB-LFP	LIB-NMC622	LIB-NMC811	LSB	ASSB-NCA	ASSB-LFP	ASSB-NMC622	ASSB-NMC811	ASSB-LSB
Cathode	Thickness	38 μm	57 μm	43 μm	36 μm	120 μm	120 μm	120 μm	120 μm	120 μm	120 μm
	AM	96%	96%	96%	96%	70%	79%	79%	79%	79%	65%
	Binder	2%	2%	2%	2%	10%	2.8%	2.8%	2.8%	2.8%	5%
	CA	2%	2%	2%	2%	20%	1.4%	1.4%	1.4%	1.4%	10%
	SEM	-	-	-	-	-	16.8%	16.8%	16.8%	16.8%	20%
Separator	Thickness	20 μm	20 μm	20 μm	20 μm	20 μm	20 μm	20 μm	20 μm	20 μm	20 μm
	Separator	100%	100%	100%	100%	100%	97.44%	97.44%	97.44%	97.44%	97.44%
	Binder	-	-	-	-	-	2.56%	2.56%	2.56%	2.56%	2.56%
Anode	Thickness	48 μm	57 μm	48 μm	50 μm	57 μm	36 μm	26 μm	32 μm	38 μm	99 μm
	AM	98%	98%	98%	98%	100%	100%	100%	100%	100%	100%
	Binder	2%	2%	2%	2%	-	-	-	-	-	-
Positive current collector	Thickness	15 μm	15 μm	15 μm	15 μm	15 μm	15 μm	15 μm	15 μm	15 μm	15 μm
Negative current collector	Thickness	10 μm	10 μm	10 μm	10 μm	10 μm	10 μm	10 μm	10 μm	10 μm	10 μm

AM: active material; CA: carbon additive; SEM: solid electrolyte material

Table 2 shows the mass distribution of components to the batteries calculated with the default and extended BatPaC. The ASSB-LSB has the lowest mass, while the LIB-LFP has the highest mass. It also shows that the batteries with sulfur as the positive active material require more cells than the other batteries due to a lower nominal voltage. Furthermore, the cathode and the anode strongly influence the mass of the battery packs. However, the cathode has a smaller influence on the batteries with sulfur as positive active material. Moreover, it is shown that the substitution of graphite as negative active material with lithium metal leads to a mass reduction due to the higher specific energy of lithium. In addition, the packaging of the battery pack can significantly increase the mass of the battery pack. Besides, the liquid electrolyte and the cooling system of the LSB have a stronger influence on the total mass than in the other batteries with liquid electrolytes, which is a consequence of the liquid electrolytes used and the number of cells required per battery pack.

Table 2 - Distribution of mass fraction to battery components in kg

Component	LIB-NCA	LIB-LFP	LIB-NMC622	LIB-NMC811	LSB	ASSB-NCA	ASSB-LFP	ASSB-NMC622	ASSB-NMC811	ASSB-LSB
Positive electrode paste	113.71	150.66	123.97	105.20	47.03	138.83	183.93	151.21	128.43	54.14
Positive current collector	20.49	22.86	20.12	20.16	11.59	9.77	15.27	10.79	9.25	7.23

Negative electrode paste/material	73.77	86.41	72.40	74.90	16.10	8.88	9.95	8.69	8.72	17.35
Negative current collector	47.59	53.09	46.76	46.85	27.53	22.99	35.72	25.35	21.80	17.38
Liquid Electrolyte	38.04	58.65	38.83	34.96	63.01	0.00	0.00	0.00	0.00	0.00
Solid electrolyte	0.00	0.00	0.00	0.00	0.00	17.85	27.99	19.72	16.86	13.06
Separator	8.82	9.86	8.66	8.67	4.95	0.00	0.00	0.00	0.00	0.00
Cell Container	20.72	26.93	21.28	20.75	25.12	17.35	23.52	18.45	16.97	20.68
Cell supervision circuit	3.07	3.52	3.17	3.17	5.44	3.07	3.52	3.17	3.17	5.44
Module packaging	22.77	30.09	23.79	22.69	23.27	17.43	24.07	18.84	17.01	18.36
Battery management system	3.52	3.60	3.54	3.54	3.93	3.52	3.60	3.54	3.54	3.93
Pack packaging	57.00	71.01	58.62	57.02	72.01	49.04	63.20	51.25	48.61	63.58
Cooling	20.26	25.68	20.59	20.52	60.41	0.00	0.00	0.00	0.00	0.00
Total	429.76	542.36	441.72	418.43	360.38	288.72	390.77	311.01	274.36	221.15

S1-1.1.2 Definition of locations and transports

It is assumed that the battery production takes place in Germany, Salzgitter. In the case of component production, the assumed locations of the unit processes are located in China except for the solid electrolyte and positive active material, which are produced in Germany, Schwarzheide. Since the production sites of the components and batteries are spatially separated, the transport distances have to be calculated. The transport of the goods is considered by the transport distances determined via the Searates¹ website. In the case of the foreground system, trucks are used for land transportation, while container ships are considered for sea transportation.

S1-1.1.3 Production process

Due to the different compositions of the investigated battery types, different production processes are carried out. The underlying production processes for the LIBs, LSB, and ASSBs are depicted in Figure 1 (Duffner et al., 2021; Kwade et al., 2018; Nelson et al., 2019; Schnell et al., 2018; Schnell et al., 2019).

¹ <https://www.searates.com/>

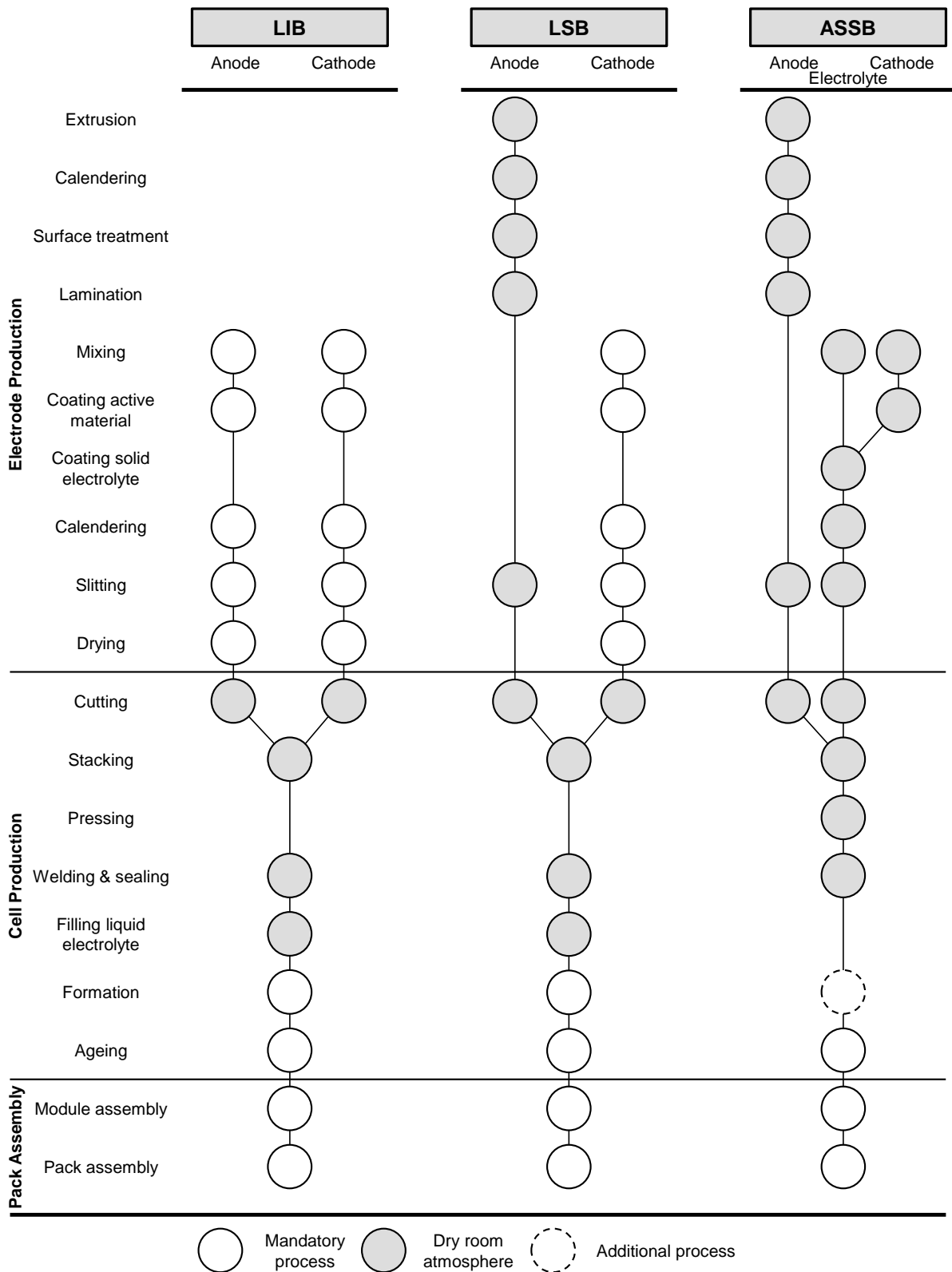


Figure 1 - Production steps of the battery technologies

The production of the battery pack, in general, can be divided into three steps: electrode production, cell production, and pack assembly (Duffner et al., 2021; Kwade et al., 2018). Since these authors already explain the production processes in detail, we will focus on the significant differences, as depicted in Figure 1. The first significant difference between the three battery technologies is the anode production. While the anode based on graphite follows similar production steps as the cathode of LIBs and the LSB, the anode based on lithium metal

includes the steps of extrusion, calendaring, surface treatment, and lamination as described by Deng et al. (2017), Schnell et al. (2018), and Duffner et al. (2021). Furthermore, these anodes with lithium metal must be produced under dry room conditions (grey shaded) due to the high moisture sensitivity of the materials used. The solid electrolyte is mixed, similar to the active material of the cathode. After the coating process of the cathode, the solid electrolyte is coated on the cathode material. The downstream processes of the electrode production are similar to the other batteries' cathode production, except that no drying is necessary before the cell production, which is a consequence of the requirement to produce all parts of the electrodes in a dry room atmosphere for the ASSB. The cell production and pack assembly processes of the LIBs and the LSB are comparable. However, they could differentiate in the requirements for the used materials, e.g., for the cutting process of the anodes. The ASSBs show more differences. First, we need a pressing process to ensure the ion conductivity and the connection between the different layers. Furthermore, no electrolyte filling is necessary because the solid electrolyte is already included in the previous steps. In addition, the formation process at the end of cell production is an optional step. For ASSBs, this step is not necessary since no solid electrolyte interface must be built. However, it is included in the assessment of the batteries since quality checks can be conducted in that process (Deng et al., 2017; Duffner et al., 2021; Kwade et al., 2018; Schnell et al., 2018).

Besides these differences, all production processes have in common that the coating process of cathodes with NMP as solvent is accompanied by solvent recovery. 99.5% of the solvent is recovered and reused in the process. Furthermore, a yield is considered during electrode and cell production (Nelson et al., 2019). The yield for the different production steps is shown in Table 3. The considered yield affects the materials required to produce 100.000 packs per year. Therefore, the additional inputs are allocated to the respective unit processes.

Table 3 - Yield of cell production

Component name	Effective yield across all steps [%]	Effective yield during mixing [%]	Effective yield during coating [%]	Effective yield during electrode slitting [%]	Effective yield during cell stacking [%]	Effective yield during electrolyte filling [%]
Cell	95					
Positive electrode material (dry)	92.2	99	95	99	99	
Negative electrode material (dry)	92.2	99	95	99	99	
Positive current collector (aluminum foil)	90.2		99	92	99	
Negative current collector (copper foil)	90.2		99	92	99	
Separators	98				98	
Electrolyte	99					99
Binder solvent recovery	99.5					

S1-1.1.4 Electricity demand

The main source to calculate the energy demand for cell production is based on Deng et al. (2017), who have calculated a range of the energy demand for large-scale production of lithium-ion batteries and LSBs. The values from the range are selected to represent current findings in the literature, such as in Degen and Schütte (2022) and Jinasena et al. (2021). For the specific production steps of ASSBs, a comparable energy demand as for LIBs and LSBs is assumed, provided that the process steps are comparable, as in mixing or coating. For those processes, which are ASSB-specific, the energy demand is approximated with the data from Keshavarzmohammadian et al. (Keshavarzmohammadian et al., 2018). Furthermore, for

the formation process, the data of Sun et al. (2020) are used, while the energy demand for the battery module and pack assembly is based on Yuan et al. (2017).”

Table 4 shows how much electricity (kWh_{el}) is required to generate one kWh battery pack capacity (kWh_p). The electricity demand increases when solid electrolytes are used, related to the increased demand for the drying room and the drying processes after coating. The difference between the LSB and the ASSB-LSB is smaller compared to the LIBs with liquid and solid electrolytes because the production of the LSB has a higher electricity demand due to the production conditions. The other differences between the LIB technologies are mainly a result of the drying process. The division of the electricity demand to the respective unit processes can be seen in supporting information 2.

Table 4: Calculated kWh_{el} for battery pack production per kWh_p

Battery type	Electricity demand [kWh _{el} /kWh _p]
LIB-NCA	53.54
LIB-LFP	61.08
LIB-NMC622	54.60
LIB-NMC811	52.83
LSB	59.05
ASSB-NCA	84.33
ASSB-LFP	105.62
ASSB-NMC622	86.43
ASSB-NMC811	81.01
ASSB-LSB	70.62

S1-1.1.5 Cost calculation in the foreground system

To estimate the cost related to the battery production, the BatPaC is used. The considered cost categories in the BatPaC comprise depreciation of machinery and buildings, personnel cost, electricity cost, material cost, "general, sales, and administration" cost, "research and development" cost, warranty cost, and overhead. Furthermore, a margin is included. However, some adaptations have been made to the BatPaC. Since the production site is located in Germany, the personnel cost rate is changed to \$43.43² per hour, and the price per square meter needed to calculate the investment into the building is changed to \$2646.18 per square meter (Turner & Townsed, 2020). Furthermore, the electricity cost of battery production is calculated as an individual cost category. The underlying price for the German electricity mix is based on the statistic of Eurostat³ for non-household consumers, which is \$0.1971 per kWh. Furthermore, the BatPaC is adapted to calculate the costs for the ASSBs and LSB. Since the machines required for the production processes, as well as the dry room conditions for LSB and ASSB, change compared to the default settings, corresponding steps are included in the cost calculation. The assumptions for investment, space, and personnel requirements are based on the default BatPaC. Process steps that are no longer required are deleted.

In contrast, the cost of the components is calculated using a top-down approach rather than a bottom-up approach compared to battery production. This means that the cost for the required input materials is deducted from the respective component's price, which is mainly based on the BatPaC. However, since the BatPaC does not include data for materials such as lithium metal or the solid electrolyte, the respective prices are added based on market data.

S1-1.1.6 Addition of sectoral exchange flow

A country-specific sectoral exchange flow is added to each unit process in the foreground system to calculate the indicator scores for the social impact categories. The particular country is selected according to the definition of the unit process, while the sector itself depends on the type of unit process that best describes the industry in which the unit process is carried

² https://ec.europa.eu/eurostat/databrowser/view/lc_lci_lev/default/table?lang=en

³ https://ec.europa.eu/eurostat/databrowser/view/NRG_PC_204_custom_4014808/default/table?lang=en

out (e.g., minerals, chemicals, metal products, machinery). For this purpose, the additional database SHDB is used to provide the background information on the risk level of different country-specific sectors. Further information on this approach and the SHDB can be found in Benoit-Norris et al. (2012), Norris and Norris (2015), and Norris et al. (2020).

S1-1.2 Intermediate system

The intermediate system comprises the life cycle inventories (LCIs) for material extraction and refinement, electricity and heat generation, and the transport processes required to describe the unit processes of the foreground system. These LCIs are mainly based on the data of the ecoinvent 3.8 database (Wernet et al. 2016). However, they are extended to allow economic and social assessment.

For the social assessment, a country has to be defined for the intermediate system's unit processes to assign a country-specific sector. For this purpose, it is assumed that material extraction and refinement take place in those countries where the production rates of the respective materials are highest (USGS, 2020). In all cases, this can be done except for the unit process "cobalt hydroxide". Since the Democratic Republic of Congo is not included in the social hotspot database, Zambia is used as an approximation to assess the social risks. Furthermore, several country-specific unit processes are created for electricity and heat generation and transportation processes, which are necessary to describe the inputs of the remaining unit processes.

For the economic assessment, an economic exchange flow ("value added") is added to the unit processes of the intermediate system. In most cases, this value added reflects the direct price of the materials or processes based on literature or market data. However, some exceptions exist for aluminum, cobalt, copper, lithium, manganese, and nickel. Since it is assumed that the extraction and refining of these materials take place in different countries, the ecoinvent processes are changed to country-specific processes. In addition, to reflect the different production steps of these materials, a top-down approach is used for the value added, similar to the component production in the foreground system.

Furthermore, individual transport distances are calculated using the Searates website for these materials. The transport distances and modes in the remaining cases are based on the ecoinvent default transport data (Borken-Kleefeld and Weidema, 2013).

Moreover, not all materials required as inputs in the unit processes in the foreground system are included in the ecoinvent databases. In these cases, approximations published in the literature are used to describe the production of these materials. The references are highlighted in the supporting information 2, including the LCIs for the intermediate system.

S1-1.3 Background system

The background system includes the data of the external ecoinvent 3.8 database and the Social Hotspots Database (Norris and Norris, 2015; Wernet et al., 2016). The unit processes of these databases are used as inputs in the intermediate and foreground systems. Furthermore, the background system consists of literature and market data, which are used to calculate the value added of each unit process in the intermediate and foreground systems.

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