Comparative Life Cycle Assessment of Battery Storage Systems for Stationary Applications

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1. Favorable characteristics of battery technologies.

Figure S1. Placement of energy storage options with respect to their power rating and discharge duration capacities. Please note that these classifications are just for general comparative purposes (at conceptual level). The sizes and discharge durations for many of the options may have broader range than shown here. Reprinted from Dunn, B.; Kamath, H.; Tarascon, J.M. Electrical energy storage for the grid: A battery of choices. Science. 2011, 334 (6058), 928–935. Copyright 2011 The American Association for the Advancement of Science.¹

Figure S1 locates various energy storage options according to their characteristics in terms of power rating and discharge duration at the rated power, along with giving some indications on their application level, i.e., power quality, load shifting and bulk power management. A closer look at the figure shows that the power ratings and discharge ranges covered by different battery technologies are very diverse in comparison with the other technological options. In addition, the following favorable characteristics of batteries, such as, high cycle efficiency, low maintenance and no tail pipe emissions at operation ends, long cycle life, compact size, modularity and scalability make them very promising candidates for stationary applications. Further, there is a considerable synergy between the battery applications for automotive and stationary purposes. This synergy combined with their modular and scalable nature provides the promise of significant cost reductions for battery technologies in the upcoming years.¹

2. Functional Unit and Comparative life cycle assessment boundaries.

2.1 Functional Unit (FU).

The perspective of this analysis is that batteries (in conjunction with power sources) allow for a functionality roughly equivalent to distributed power supply options. Thus, they can't be treated just as storages, as they are competing with other distributed conventional power supply options like diesel/natural gas generators nowadays (see Table S1 listing a couple of competing distributed power generation technologies). The decision to install a grid-connected battery system might directly/indirectly be a decision not to install any of these distributed generation technologies. In addition, batteries once installed in an electricity network (for e.g., to store grid electricity for energy management at community scale) act as any other normal electricity from the corresponding power sources. The point to be noted here is that batteries don't have independent existence in the electricity network, i.e., they always exist as conjugated systems with power sources. Hence, a decision to install batteries will directly influence the impacts of associated power source which in conjunction will govern the overall impacts arising from

taking such a decision. Thus, it becomes inevitable to account for complete impacts arising from battery + power source conjugate system to get a real insight into the overall environmental impacts arising from battery installations; accounting for just electricity losses due to batteries or viewing batteries in isolation as done in previous studies (the prevalent trend in literature) won't help in comparing them with their competitors or even to get an idea about the overall environmental burdens to deliver 1 MWh of electricity via batteries.

The battery centric analyses are very much important as well, but they analyze batteries in isolation and will help in taking microscopic decisions about batteries (for e.g., in identifying hotspots in the battery life cycle only). But these kinds of analyses will be of little help when a decision maker asks systemic questions, for example (among others), how environmental friendly is installing batteries when compared to installing and running micro/small scale natural gas/diesel generators for community energy management (or load shifting, etc)? How much environmental friendly is installing batteries with solar PVs in comparison to grid-connected ones? What is the break-even point for the impacts of grid-electricity so that the impacts of grid-connected batteries shall not exceed the present environmental load? How much penetration of renewable energies is required so that the integrated impacts of batteries & grids will not cross over the present environmental load?

Thus, the authors attempt in this manuscript is to go towards providing that complete figure (i.e., overall impacts arising from battery + power source system to deliver 1 MWh electricity) which is really needed in decision making process (say, in making a decision to deploy huge numbers of large scale grid-connected batteries towards which Japanese and German governments are heading; in such a context, it will be totally misleading to define a FU that looks at batteries only in isolation).

Moreover, this FU helps in comparing the environmental advantage of batteries under different application scenarios wherein the power sources change (for e.g., we use solar electricity in self-consumption stationary application whereas grid electricity in other scenarios) and also in studying the impacts of changing power mixes on battery ranking to highlight the potential environmental advantage in making transition towards future greener grids (for e.g., in section "Sensitivity Analyses - Power-Grid Mix").

Example case: Calculating environmental advantage of charging Li-Ion batteries with solar versus grid electricity using the two FUs

FU₁ considering only impacts of battery electricity losses in use stage:

GWP advantage in charging Li-Ion battery with grid versus solar = Li-Ion (with solar) – Li-Ion (with grid) = 19 - 83 = -64 kg.CO₂eq./MWh

FU₂ considering impacts of electricity stored in use stage (used in this study):

GWP advantage in charging Li-Ion battery with grid versus solar = 105 - 748 = -643 kg.CO₂eq./MWh

Thus, FU_1 under-estimates the GWP advantage of charging Li-Ion batteries with solar instead of grid by nearly 10 times the estimation provided by FU_2 .

This example might be a very simplistic case of having batteries in today's grids compared to the future grids wherein the penetration of renewable energies will be very high. Given the synergy between batteries and renewable energies, the case for installing batteries to make a transition towards highly renewable-grid scenario via FU_2 will become stronger than the one via FU_1 as the former shows more potential advantage than the latter.

2.2. Comparative life cycle assessment boundaries.

Figure S2 shows a schematic of the life cycle stages considered in this study, along with highlighting some of the major components across each life cycle stage. The transportation activities are taken into account in the cradle to gate values (i.e., transportation during component and product manufacturing stages and upstream processes), but are excluded in the analysis after this stage (i.e., product distribution stage is not included in the modeling). This is mainly because it is assumed that these values will be similar for all the four kinds of technologies studied and hence will not play a major role in the comparative analysis of the same.

Further, as the main focus of the study is on the use stage of the battery technologies, the impacts of electricity generation and transmission arising from charging batteries in the use stage are considered in the analysis. But, energy, resources and materials required for upstream processes for supporting infrastructure and to manufacture battery accessories – among others – converters, battery support structures and wiring are not included as these are assumed to be similar for all the four technologies. The study uses most of the data from the LCA literature applicable to European countries. The batteries are assumed to be deployed in Germany and the German distribution grid mix from Ecoinvent 3.01 database² is assumed. In the second stage of the analysis for lithium-ion (Li-Ion), the batteries are assumed to be manufactured in Europe and used in Germany. But, the manufacturing of individual battery components may take place outside Europe (e.g., China); this is also true for resource extraction (e.g., Chile for Lithium & Congo for Cobalt) and other upstream processes.

Technology	Application range	Electric conversion efficiency	Application	Fuel	Comments
Reciprocating Engines	Diesel: 20kW-10+MW Gas: 5kW-5+MW	 Diesel: 36% - 43% Gas: 28% - 42% 	Emergency or standby Services & CHP	 Diesel, also heavy fuel oil and bio-diesel Gas, mainly natural gas, biogas and landfill gas can also be used 	By far most common technology below 1MWe
Gas turbines	1 - 20MW	21% - 40%	CHP & Peak power supply units	Gas, kerosene	
Micro turbines	30kW -1MW (also, small scale up to < 1 kW)	25% - 30%	Power generation, possible with CHP added	Generally uses natural gas, but flare, landfill and biogas can also be used	
Fuel cells	1kW-5MW	35%-60% (Electric efficiency of small-scale applications ~25%)	Transport, stationary use and power generation (CHP & UPS)	Methanol, Hydrogen or natural gas (Reforming of CH ₄ to H ₂ leads to decreased efficiency)	The ranges include all types of fuel cells (individual application ranges of each fuel cell technology might vary considerably)

Table S1. Distributed generation technologies and characteristics (data/information from Pepermans et al.).¹⁷



Figure S2. Life Cycle stages modeled in this study (assessment boundaries).

3. Modeling Methodology and Life Cycle Inventory analysis.

The modeling methodology adopted to quantify the life cycle impacts of batteries is as follows. First, the cradle-to-gate LCI data per kilogram of battery material or MWh of battery capacity, the battery characteristic data and the stationary application characteristic data were collected. Second, battery system sizing was carried out by taking into account the required application energy rating and the losses that occur during one complete charge-discharge cycle; the DOD of the batteries was set to 80% to avoid deep discharging. Third, the number of batteries required for a service life of 20 years was calculated for each application scenario; this depends on the calendrical and cycle life of batteries plus the number of cycles demanded by the stationary application over a 20 year period. Fourth, the cradle-to-gate impacts of batteries resulting from the delivery of 1 MWh_d of electricity were calculated by normalizing the values for 20 years or until the end of their useful life. Finally, the impacts from electricity losses and associated power sources during the use stage were calculated and then added to the cradle-to-gate values in order to estimate the life cycle impacts from the delivery of 1 MWh_d of electricity. In addition, to account for uncertainties in the input data, worst and best case scenarios were estimated and sensitivity analyses were carried out (see Figure S3).

3.1. Equations and calculation tables

Abbreviations: c2g = cradle-to-gate; DoD = Depth of Discharge

Constants:

application_energy_MWh = required end user energy rating per cycle (varies with different application requirements)

round_trip_efficiency = average, high and low values taken from Table S4

energy_density_MWh_per_kg = taken from Table S4

DoD = 80% in all scenarios, except for 'Area & Frequency regulation' application scenario (5%, see table)

cycles = cycle life of battery at 80% DoD

cycles_application = number of cycles demanded by a application in 20 year time scale

calendrical_life = material lifetime of a battery after which it becomes unusable

c2g_impact_of_battery_MJ_per_kg = values from literature (Table S3)

electricity_impact_MJ_per_MWh = values from ecoinvent 3.01 (see Table S2)

no._batteries_20_years = no. of batteries used in 20 years time scale = 20 / calendrical_life (if application cycles demanded is less than the battery cycle life within its calendrical lifetime); else = cycles_application / cycles (if application cycles demanded is more than the battery cycle life within its calendrical lifetime)

Equations:

system_size_MWh = battery capacity installed (MWh_installation.capacity) =
application_energy_MWh * round_trip_efficiency^{-0.5} * DoD^{-1}

mass_battery_kg = system_size_MWh / energy_density_MWh_per_kg

<u>c2g for complete battery utilization:</u>

lifetime_electricity_delivered_MWh = application_energy_MWh * cycles

c2g_impact_battery_MJ_per_MWh = (mass_battery_kg) * (c2g_impact_battery_MJ_per_kg) / (lifetime_electricity_delivered_MWh)

<u>c2g for battery utilization in different applications:</u>

lifetime_electricity_delivered_applications_MWh = application_energy_MWh * cycles_application

{Cycles = cycle life (at 5% DoD for 'Area & Frequency regulation' application scenario; for all others 80% DoD)}

c2g_impact_battery_MJ_per_MWh = (mass_battery_kg) * (c2g_impact_battery_MJ_per_kg) * (no._batteries_20_years) / (lifetime_electricity_delivered_applications_MWh)

use.phase_impact_battery_MJ_per_MWh = electricity_impact_MJ_per_MWh / round_trip_efficiency

total_Impacts_battery.power.supply_MJ_per_MWh = c2g_impact_battery_MJ_per_MWh + use.phase_impact_battery_MJ_per_MWh

MODELLING METHODOLOGY (ISO 14040 & 14044)

GOAL & SCOPE DEFINITION

Goal of the study, Functional unit, Product systems, Assessment boundaries, Data management and Data quality

LIFE CYCLE INVENTORY (LCI)

Modeling Cradle-to-gate LCA Stages

- 1. Generic LCI data collection for all four battery technologies
- 2. Detailed LCI data collection for Lithium Ion process chains

Use Stage Battery characteristic data Round-trip Efficiency, Cycle Life and Calendrical Life Application characteristic data Required power rating, Required Energy rating, Discharge duration & Cycle frequency

Battery System Sizing Six Stationary Application Scenarios

Characterizing Electricity Consumption

LIFE CYCLE IMPACT ASSESSMENT (LC	IA)
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Impact Categories Cumulative Energy Demand (CED) Global Warming Potential (GWP)	 Impacts to deliver 1 MWh of useful electricity Cradle-to-gate impacts of battery Impacts from battery use stage Life Cycle Impacts 					
ReCiPe 2008 Worst Sensiti	and Best Case Scenarios vity Analyses					
INFERE	NCES and IMPLICATIONS					

Figure S3. LCA modeling methodology used in the study.

Sl. No.	Process	CED (MJ/MWh)	GHG (kg.CO ₂ -eq. /MWh)	Comments
1.	Electricity, low voltage {DE} market for Alloc Def, U	11,000	665	Average German mix at low voltage grid
2.	Electricity, production mix photovoltaic, at plant/DE U	4,950	86.5	Average German PV production mix
3.	Electricity, at wind power plant/RER U	4,000	11.2	Average EU geographical mix
4.	Natural gas, at plant/DE U	113	563	Typical natural gas power plant located in Germany

Table S2. CED and GHG impacts of power sources (values from Ecoinvent 3.01).

Table S3. Cradle-to-gate CED and GHG impacts of the battery types.

Battery types	CED (MJ/kg)	GHGs (kgCO2eq./kg)	References	comments
Li-Ion	196	22	Majeau- Bettez(2011) ³	CED estimated by authors based on Majeau- Bettez(2011)
PbA	39.6	2.7	Spanos et.al	
PbA-R (30/70)	32.7	1.9	(2015) ¹⁵	Estimated from Tables 5, 6, 13 & 19
NaS	180.7	14.9	Sullivan(2012) ⁹	Average values (Table 7, Figures 6 & 7)
V-Redox	37.5	2.7	Denholm(2004) ¹⁶	Estimated from Tables 6,7,8 & 9 (assumed energy density of 20 Wh/kg)

Table S4. Battery characteristic data used in the LCA simulation (data primarily based on Battke et al.⁶ unless noted).

Round-trip EfficiencyBattery(%)Type(%)				Cycle life (no. of cyc	at 80% D cles to fai	OD lure)	Energy density ^a (Wh/kg)	Calendrical life ^d
	Average	Low	High	n Average Low High				
Li-Ion	90	85	98	10250	5000 ^c	15000 ^c	140	11.5
PbA	82	80	90	1250	1000 ^c	1500 ^c	27	8.5
NaS	81	71	90	3333	2500	5000	116	8.5
V-Redox	75	60 ^b	80	13000	10000	15000	20	9.5

a – Energy density values taken from: Li-Ion – Majeau-Bettez et al.,³ PbA – Spanos et al.,¹⁵ NaS & V-Redox – Rydh and Sanden.¹⁰

b – Data taken from Rydh and Sandén.¹⁰

c – Upper and lower bound values from Battke et al.⁶

d – Average values from Battke et al.⁶

Note:

1. By default, the average values were used in the simulations; high and low values were used in generating worst and best case scenarios and in sensitivity analyses.

2. Cycle life @ 5% DOD was assumed for Area & Frequency regulation application scenario; the corresponding values assumed are 53733, 6378, 24505 and 22730 for Li-Ion, PbA, NaS & V-Redox, respectively.

	Required	Discharge	Required	Cycle
Application	Power Rating	Duration	Energy Rating ^a	Frequency ^b
	(MW)	(h)	(MWh)	(cycles/day)
Energy Management	0.1	2.5	0.25	2 (14600)
(community scale)				
Increase of Self-	0.0025	4	0.01	0.6 (4380)
Consumption				
Area and Frequency	2	0.25	0.5	$34(248200)^{c}$
Regulation				
Support of Voltage	1	0.25	0.25	0.68 (4964)
Regulation				
T&D Investment Deferral	10	5	50	0.68 (4964)
Utility Energy Time-Shift	100	8	800	1 (7300)

Table S5. Input data for stationary application scenarios (data primarily based on Battke et al.⁶).

^{a.} It was assumed during the simulation that this much amount of energy was withdrawn from the battery during each cycle (except for Area & Frequency Regulation).

^{b.} The values in brackets show the number of cycles required for 20 years of service.

^{c.} For this application, it was assumed that the energy equivalent to only 5% DOD of corresponding battery size was withdrawn during each cycle. This is because of the requirement from European Network of Transmission System Operators for Electricity (ENTSO-E) for storage devices to be available for 15 minutes for Area and Frequency Regulation application even-though the storage devices operate only for 38 seconds on an average as estimated by Battke et al. (2013). Thus, the battery storage is used around 5% DOD for most of the time (38 seconds out of 15 min equals 4.2%).

Battery	Application	System	no.	C2g CED	Total CED	C2g GHG	Total GHG
type	Energy	Size	of	impacts	impacts	impacts	impacts
	(kWh)	(kWh)	batte	(MI/MWha)	(MI/MWha)	$(kgCO_2eq.$	(kgCO ₂ eq./
			ries*			$/N W N_d$	$\mathbf{W} \mathbf{W} \mathbf{n}_{d}$
Scenario: C	Complete utiliz	ation of batter	ries	I	I	I	I
Li-Ion	1000	1318	NA	180	12402	20.2	759
PbA	1000	1380	NA	1622	15036	109.9	921
PbA-R	1000	1380	NA	1340	14753	76.9	888
NaS	1000	1389	NA	649	14229	53.5	874
V-Redox	1000	1443	NA	208	14874	14.8	901
Scenario: In	ncrease of Self	-Consumption	n	I	I	I	I
Li-Ion	10	13.2	1.7	732	6232	82	178
PbA	10	13.8	3.5	1622	7658	110	215
PbA-R	10	13.8	3.5	1339	7376	77	182
NaS	10	13.9	2.3	1162	7273	96	203
V-Redox	10	14.4	2.1	1300	7900	93	208
Scenario: E	Energy Manage	ment (comm	unity sc	ale)			
Li-Ion	250	329	1.7	220	12442	25	763
PbA	250	345	11.7	1622	15036	110	921
PbA-R	250	345	11.7	1339	14754	77	888
NaS	250	347	4.4	649	14229	53	874
V-Redox	250	360	2.1	390	15057	28	914
Scenario: T	&D Investmer	nt Deferral	1	1	1	1	1
Li-Ion	50000	65881	1.7	646	12868	72	811
PbA	50000	69020	4.0	1622	15036	110	921

Table S6. Intermediate results (Average values).

PbA-R	50000	69020	4.0	1339	14754	77	888			
NaS	50000	69444	2.3	1025	14606	84	905			
V-Redox	50000	72169	2.1	1147	15814	82	968			
Scenario: Utility Energy Time-Shift										
Li-Ion	800000	1054093	1.7	439	12662	49	12271			
PbA	800000	1104315	5.8	1622	15036	110	13524			
PbA-R	800000	1104315	5.8	1339	14754	77	13491			
NaS	800000	1111111	2.3	697	14278	57	13638			
V-Redox	800000	1154701	2.1	780	15447	56	14722			
Scenario: S	Support of Vol	ltage Regulati	on							
Li-Ion	250	329	1.7	646	12868	72	12295			
PbA	250	345	4.0	1622	15036	110	13524			
PbA-R	250	345	4.0	1339	14754	77	13491			
NaS	250	347	2.3	1025	14606	84	13665			
V-Redox	250	360	2.1	1147	15814	82	14748			
Scenario: A	Area and Freq	uency Regula	tion							
Li-Ion	500	659	4.6	549	12771	62	12284			
PbA500	500	690	38.9	5085	18500	344	13759			
PbA-R	500	690	38.9	4199	17614	241	13656			
NaS	500	694	10.1	1413	14993	116	13697			
V-Redox	500	722	10.9	1904	16571	136	14802			

* number of batteries consumed in 20 years service time (not applicable in case of "complete utilization of batteries" scenario)

3.2. Life cycle inventory (LCI) for qualitative analysis of Li-Ion process chains.

The detailed inventories were built for three different Li-Ion chemistries: Iron Phosphate (LFP), Nickel Cobalt Manganese (NCM) and Manganese Oxide (LMO). Table S1 summarizes the materials and their percentages component wise for typical Li-Ion batteries. The data for manufacturing stage processes is completely taken from Majeau-Bettez et al.,³ with only exception of LMO wherein the data for positive electrode material comes from Notter et al.⁴ It should also be noted that both of these studies rely primarily on Ecoinvent 2.2 database² for background data on upstream processes and materials extraction stages. Thus, apart from manufacturing stage processes, rest of the LCI data for our study comes from Ecoinvent 2.2 database². Table S2 provides a list of materials and processes involved in the manufacturing of LFP, along with data values used in the LCA modeling (summary of cradle-to-gate stage). Similar data tables with minor modifications in some of the key materials and processes were generated for the other two Li-Ion chemistries, NCM & LMO as well (see Table S3 and Table S4). For complete detailed inventory on sub-processes, the reader is suggested to go through Majeau-Bettez et al.³ and Notter et al.⁴ supporting information sheets.

Table S7: Components and materials of a typical Lithium-Ion battery.

Components	Percentage*	
Components	(Typical)	
Anode	15 – 24	
Copper foil (electrode substrate - negative)	1 – 12	
Battery grade graphite/carbon (Negative electrode material)	8 – 13	
Polymer (Binder)	<1 - 10	
Auxiliary solvent	<1-6	

Cathode	29 – 39
Aluminum (electrode substrate - positive)	4 – 9
Positive electrode material	22 – 31
Lithium manganese oxide (LMO-Spinel)	
Lithium-nickel cobalt manganese oxide (Li-NCM)	
Lithium iron phosphate (LFP)	
Polymer/other (Binder)	<1 - 3
Auxiliary solvent	<1 - 11
Separator	2 – 3
Polymer (Polyolefin)	2 – 3
Cell Casing	3 – 20
Aluminum casing and pouch material (Polypropylene resin)	3 – 20
Electrolyte	8 – 15
Carbonate solvents (Ethyl carbonate, Lithium fluoride, Phosphorus pentachloride, Lithium chloride extraction)	7 – 13
Lithium hexa-fluorophosphate (LiPF6)	1 – 2
Battery Management System (BMS)	2
Copper wiring	1
Steel	1
Printed wire board	<1
Battery Pack Casing/Housing	17 – 23
Polypropylene/polyethylene terephthalate	17 – 23
Steel (housing material)	
Passive Cooling System	17 – 20
Steel and aluminum (sheet metals)	17 – 20
Total	100
* Typical values taken from Shanika Amarakoon et al. ⁵	

Table S8: Summary of manufacturing processes for LFP and its sub-components (data primarily based on Majeau-Bettez et al.;³ check the source for more details on sub-inventories).

Products	Amount	Unit
Lithium Ion Battery (LFP)	1	kg
Materials/fuels	I	1
Positive electrode material for Li-Ion (LFP) at Plant (dry)	0.25	kg
Negative electrode material for Li-Ion battery at Plant (dry)	0.08	kg
Li-Ion electrode substrate (positive), at plant	0.036	kg
Li-Ion electrode substrate (negative), at plant	0.083	kg
Electrolyte for Li-Ion Battery, 1M LiPF6	0.12	kg
Separator material for Li-Ion, at plant	0.033	kg
Cell container (Li-Ion), at plant	0.2	kg
Module and battery packing	0.17	kg
Battery management system for Li-Ion battery	0.02	kg
Water, decarbonised, at user {RER} water production and supply, decarbonised Alloc Def, U	380	kg
Electricity/heat		1
Electricity, medium voltage, production UCTE, at grid/UCTE U	27	MJ
Heat, light fuel oil, at industrial furnace 1MW/RER U	2.9	MJ
Heat, natural gas, at industrial furnace low-NOx >100kW/RER U	22	MJ
Transport, freight, rail/RER U	0.23	tkm
Transport, lorry >16t, fleet average/RER U	0.051	tkm
Facilities precious metal refinery/SE/I U	1,9*10^-8	р
Emissions to air	1	1
Heat, waste	52	MJ

Table S9: Summary of manufacturing processes for LMO and its sub-components (data primarily based on Majeau-Bettez et al.;³ only positive electrode material is based on Notter et al.⁴; check the sources for more details on sub-inventories).

Products	Amount	Unit
Lithium Ion Battery - LMO	1	kg
Materials/fuels		
Positive electrode material for Li-Ion (LMO) at Plant (dry)	0.24	kg
Negative electrode material for Li-Ion battery at Plant (dry)	0.094	kg
Li-Ion electrode substrate (positive), at plant	0.036	kg
Li-Ion electrode substrate (negative), at plant	0.083	kg
ELectrolyte for Li-Ion Battery, 1M LiPF6	0.12	kg
Separator material for Li-Ion, at plant	0.033	kg
Cell container (Li-Ion), at plant	0.2	kg
Module and battery packing	0.17	kg
Battery management system for Li-Ion battery	0.03	kg
Water, decarbonised, at user {RER} water production and supply, decarbonised Alloc Def, U	380	kg
Electricity/heat	I	
Electricity, medium voltage, production UCTE, at grid/UCTE U	27	MJ
Heat, light fuel oil, at industrial furnace 1MW/RER U	2.9	MJ
Heat, natural gas, at industrial furnace low-NOx >100kW/RER U	22	MJ
Transport, freight, rail/RER U	0.23	tkm
Transport, lorry >16t, fleet average/RER U	0.051	tkm
Facilities precious metal refinery/SE/I U	1,9*10^-8	p
Emissions to air	1	1
Heat, waste	52	MJ

Table S10: Summary of manufacturing processes for NCM and its sub-components (data primarily based on Majeau-Bettez et al.³).

Products	Amount	Unit
Lithium Ion Battery - NCM	1	kg
Materials/fuels		L
Positive electrode material for Li-Ion (NCM) at Plant (dry)	0.23	kg
Negative electrode material for Li-Ion battery at Plant (dry)	0.094	kg
Li-Ion electrode substrate (positive), at plant	0.036	kg
Li-Ion electrode substrate (negative), at plant	0.083	kg
ELectrolyte for Li-Ion Battery, 1M LiPF6	0.12	kg
Separator material for Li-Ion, at plant	0.033	kg
Cell container (Li-Ion), at plant	0.2	kg
Module and battery packing	0.17	kg
Battery management system for Li-Ion battery	0.03	kg
Water, decarbonised, at user {RER} water production and supply, decarbonised Alloc Def, U	380	kg
Electricity/heat	l	
Electricity, medium voltage, production UCTE, at grid/UCTE U	27	MJ
Heat, light fuel oil, at industrial furnace 1MW/RER U	2.9	MJ
Heat, natural gas, at industrial furnace low-NOx >100kW/RER U	22	MJ
Transport, freight, rail/RER U	0.23	tkm
Transport, lorry >16t, fleet average/RER U	0.051	tkm
Facilities precious metal refinery/SE/I U	1,9*10^-8	р
Emissions to air	1	1
Heat, waste	52	MJ

3.3. Stationary applications characteristic data.

In this study, the following six stationary application scenarios were chosen for analysis based on the work of Battke et al.:⁶

- 1. *Energy Management (Community Scale)*: Here application of storage helps in managing the electricity consumption of a community by giving more flexibility to the energy demand patterns and reducing peak demand;
- 2. *Increase of Self Consumption*: Increases the self-consumption of electricity for household/small scale PV systems wherein the consumers are feeding electricity to the grid. This helps in decreasing the energy demand of the consumer and reduces the burdening of distribution grid due to excessive feeding, especially during peak generation times;
- 3. *Area and Frequency Regulation*: Maintains the grid frequency within permissible limits by absorbing short time fluctuations;
- 4. *Support of Voltage Regulation*: Helps in maintaining the power quality at a distribution grid level;
- Transmission & Distribution (T&D) Investment Deferral: Helps in deferring T&D investments by storing electricity during congestion, and also enhances the T&D system utilization factor;
- 6. *Utility Energy Time-shift*: Decouples utility's energy generation from the demand over daily time scale, for example, storing electricity during off-peak hours and discharging the same during peak hours of the day.

3.4. Electricity sources.

The LCI data for all the electricity sources comes from Ecoinvent 3.01 database² (see Table S2): *A. German national electricity grid mix (at distribution level)*: The data includes the life cycle inventory of electricity production, transmission and distribution in Germany, including the data of imported electricity from neighboring countries. Electricity losses during transmission and distribution, including the transformations from medium to low-voltage and during electricity distribution are accounted for.

B. Solar only scenario: The data takes into account the production mix of solar PV electricity in Germany. It includes the life cycle inventories of PV panels, inverters and other associated transport activities and accessories. This electricity mix is used in modeling the self-consumption application scenario and in sensitivity analyses.

C. 50% solar – 50% wind scenario: This dataset is the 50-50 average of both solar only and wind only electricity data. The solar data used is same as the one used for solar only scenario. The wind data includes the data from typical wind power plant modules used in Europe (averaged over European geography). The data also accounts for the life cycle inventories of accessories used for wind power productions and associated transport activities.

D. Natural Gas scenario: It accounts for the life cycle inventory data to produce electricity from a typical natural gas power plant located in Germany. This scenario is merely used as a reference scenario in detailed analysis of Li-Ion process chains, just for comparative purposes.

4. Life Cycle Impact Assessment (LCIA).

The LCIA phase aims to assess the inventory analysis (LCI) results and interpret the same in terms of potential environmental threats associated with the product's value chain.¹¹ In general, LCIA involves the following key steps: selection of impact categories (e.g., climate change, terrestrial toxicity); classification - attributing inventory results to impact categories (e.g., attributing carbon dioxide emissions to global warming potential (GWP)); characterization - selection of characterization models and expressing the contributions from all substances in the impact category into a common unit of the category indicator (e.g., using IPCC characterization models and summing up the impacts of all greenhouse gases (GHGs) into kg CO₂-equivalents (GWP) under the impact category of climate change); normalization – normalizing the characterization results on a common scale that applies to all impact categories (e.g., normalizing GWP score of a product by the GWP from an average per capita European lifestyle); the final steps of LCIA may include grouping and weighting of impact categories.

The impact categories considered in this study are as follows:

Cumulative Energy Demand (CED): The impact category intends to estimate the total energy used across the product's life cycle, both direct and indirect energy uses.¹²

Global Warming Potential (GWP-100): The impact category investigates the total amount of greenhouse gases (GHGs) emitted into the atmosphere across the life cycle of the product, and uses IPCC characterization model (2007) for time horizon of 100 years to estimate the global warming potential of the product.¹²

ReCiPe 2008 Methodology: This method tries to transform the long list of inventory results to 18 midpoint impact categories to 3 endpoint impact categories to one single impact score in the

end. The 18 midpoint impact categories range from ozone depletion to climate change to water consumption, and these mid-points are aggregated to 3 endpoint impact categories, such as, damages to human health, ecosystems and resource availability. It should be noted that only 17 midpoint impact categories were modeled in this study (water consumption category was left out).¹³

See Hischier et al.¹² & Goedkoop et al.¹³ for a detailed description and explanation on these impact categories, including the methodologies for quantifying the impact categories.Figure S3 summarizes the LCA modeling methodology used in the study.

5. Supplementary Results.

5.1. Cradle-to-gate impacts for different stationary applications.

The variations in the relative ranking of battery types across different application scenarios in the cradle-to-gate stage results arise primarily from the underutilization of the battery types in different applications. That is, if all the battery types are utilized completely in all the six application scenarios, then no variation in the relative ranking of battery types will be observed across different application scenarios. This becomes more evident in Figure S4 wherein the mean cradle-to-gate CED impacts of four battery types are plotted across the number of cycles demanded by the different application scenarios.



Figure S4. Dependency of Cradle-to-gate battery CED impacts on application cycles.

The following observations can be made from Figure S4. First, the CED impacts of Lithium Ion and Vanadium Redox-flow decrease drastically as the number of cycles demanded by the application scenarios increase. This is because, in all the application scenarios considered in this study, Li-Ion and V-Redox are under-utilized, i.e., their complete cycle life at 80% DOD (10250 for Lithium Ion & 13000 for Vanadium Redox-flow) are not utilized as the number of cycles demanded by the application scenarios are much lower (maximum being 14600 for 'Energy Management - community scale' for 20 years of service time). As these battery types have calendrical life of around 10 years, they would be discarded when they reach their calendrical life even-though their cycle life is under-utilized. Hence, the CED impacts of these battery types decrease with the increasing application cycles, as this means more proper utilization of cycle life and hence more electricity delivered for the same battery material. Thus, these two battery types become more competitive with the increasing application cycles. Second, the CED impacts of NaS decrease with the number of application cycles initially, and then stabilize afterwards.

This is because NaS is under-utilized in all the application scenarios except in 'Energy Management-community scale' and complete-life utilization scenarios. The CED impacts therefore decrease till 14600 cycles (Energy Management-community scale scenario) wherein its cycle life is completely utilized, and then the value stabilizes. Lastly, the CED impacts of PbA(R) show indifference to the application cycles as its cycle life (around 1250 at 80% DOD) is utilized completely in all the application scenarios. Note also that the 'Area and Frequency Regulation' application is excluded in the above discussion as it has got different assumptions compared to the other application scenarios. Hence, it cannot be compared with others directly. But nevertheless the arguments discussed will hold true for this case as well.

Further, Figure S5 shows variation of life cycle battery CED impacts (mean values) with application cycles. As mentioned in the main article, the use stage impacts which dominate the life cycle scenario have no contribution to the variations across different application scenarios. Hence, the impact of cradle-to-gate variations in the relative ranking of battery types across different application scenarios has a very minor effect on the life cycle results.



Figure S5. Variation of Life Cycle battery CED impacts with application cycles.



Figure S6. Comparative CED impact assessment of the battery types for seven different stationary applications. Top figure shows the results for only cradle-to-gate impacts, while the bottom figure shows the life cycle impacts.

5.2. Sensitivity Analysis.



Figure S7. Effect of different electricity mix scenarios on the life cycle CED impacts of batteries.

Figure S7 compares the life cycle CED impacts for three different electricity mix scenarios. It becomes quite evident that a transition towards solar and wind energy scenarios brings down the life cycle CED impacts drastically, as low as less than 50% the impacts of *German distribution grid* scenario. In addition to this, two more things happen when low carbon electricity sources such as solar and wind are used to charge the batteries; the relative share of cradle-to-gate impacts in the life cycle impacts increases and the difference in the relative ranking of the four battery types decreases.



Figure S8. Impact of changing the round-trip efficiency (left) and the cycle life (right) from the mean values used in the LCA model.

5.3. Lithium-Ion qualitative analysis.

Figure S9 shows the CED impacts of the major battery processes during the cradle-to-gate stage of Li-Ion life cycle to produce one kg of battery material at manufacturing outlet. The main contributors are – in the decreasing order – electricity used during manufacturing stage, battery management system (from using integrated circuit components), cell container (from Aluminum production), cathode (from positive electrode material), module and battery packaging (from using Polyethylene terephthalate), electrolyte (from Lithium hexa-fluorophosphate) and anode (negative electrode material such as graphite and substrate such as copper).

A similar plot for GWP impact category is shown in Figure S10. Although the main contributing processes and relative trend remain same as for CED for most of the components, a different trend is observed for positive and negative electrode materials. This is mainly because of the usage of tetra-fluoroethylene in the manufacturing of cathode and anode materials; tetrafluoroethylene contains Chloro-di-fluoromethane which results in the emissions of CFCs and HCFC gases that have very high global warming potential (CFCs have around 5000-10000 times more global warming potential than carbon dioxide, while HCFCs have around 100s-1000s times more¹⁴).



Figure S9 CED impacts of the major processes during the cradle-to-gate stage of Li-Ion battery life cycle.

Table S11: Six ReCiPe 2008 mid-point impact categories that are significantly affected by Li-Ion cradle-to-gate process chains and the corresponding key components/processes that affect them.

Mid-point impact categories	Key components/processes from cradle-to-gate stage of Li-Ion that affect the corresponding category
Climate Change – human Health	Cathode (positive) & anode (negative) electrode materials, BMS, electricity used in manufacturing processes, cell container and heat generated from natural gas
Human Toxicity	Negative electrode substrate (from copper production) and

	BMS (from copper & Integrated circuits used)
Particulate matter formation	Cathode (positive electrode material), negative electrode substrate, BMS, cell container and electricity (manufacturing)
Climate Change Ecosystems	Cathode (positive) & anode (negative) electrode materials, BMS, electricity used in manufacturing processes, cell container and heat generated from natural gas
Metal depletion	Cathode material (manganese, nickel, etc), negative electrode substrate (copper) and BMS (gold and chromium)
Fossil depletion	Electricity (hard coal), BMS (wafer & hard coal), module and battery housing (xylene), cell container (aluminum), electrolyte (ethylene), negative electrode material (graphite) and positive electrode material



Figure S10 GWP impacts of the major processes during the cradle-to-gate stage of Li-Ion battery life cycle.



Figure S11 ReCiPe 2008 single point score for Li-Ion cradle-to-gate processes that adversely impact the environment.



Figure S12 Adverse environmental impacts of Li-Ion life cycle process chains on ReCiPe midpoint impact categories (Method: ReCiPe 2008 Endpoint / Europe H/A). The Y-axis is a dimensionless parameter as the impacts are normalized to the corresponding environmental load of an average European citizen.

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