Update of Bill-of-materials and Cathode Materials Production for Lithium-ion Batteries in the GREET® Model

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FIGURES

TABLES

ACRONYMS

3C	Computer, Communication, and Consumer electronics
BatPaC	Battery Performance and Cost
BEV	battery electric vehicle
BOM	bill-of-material
CATARC	China Automotive Technology and Research Center
EV	electric vehicle
HEV	hybrid electric vehicle
LCA	life cycle analysis
LCI	life cycle inventory
LCO	lithium cobalt oxide
LFP	lithium iron phosphate
LIB	lithium-ion battery
LMO	lithium manganese oxide
NCA	lithium nickel cobalt aluminum oxide
NMC	lithium nickel manganese cobalt oxide
PHEV	plug-in hybrid vehicle

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This memo documents updates in the GREET® model for 1) bill-of-materials (BOMs) of lithium-ion batteries (LIBs) for electric vehicles (EVs), including hybrid electric vehicles (HEVs), plug-in hybrid vehicles (PHEVs), and battery electric vehicles (BEVs); 2) life cycle inventory (LCI) for the production of LIB cathode materials, including lithium cobalt oxide (LCO), lithium nickel cobalt manganese oxide (NMC), and lithium nickel cobalt aluminum oxide (NCA). The BOM update was based on the most recent version of Argonne's Battery Performance and Cost (BatPaC) model. The cathode LCI update was based on our site visit to one leading cathode material producer, literature, and industry reports. These updates therefore represent current material compositions of LIB for transportation applications and the state-of-the-art of industrial production of LIB cathode materials, and are incorporated into GREET 2018.

1 LITHIUM ION BATTERY BILL OF MATERIALS

Existing BOMs for LIBs in GREET 2017 were last updated in 2015, based on BatPaC version 2.0 (Dunn *et al.*, 2015). The LIB cathode chemistries and battery designs have evolved in recent years towards higher specific energy and lower cobalt content. The LIB characteristics are therefore updated in GREET 2018 to account for these trends. Specifically, the LCO-based LIB in GREET 2017 is superseded by one based on $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC811) in GREET 2018, as LCO-based LIBs are not currently used for traction applications, and will not be used for this application in the near future, while NMC811 has been touted as one of the next-generation cathode materials for LIBs on PHEVs and BEVs (Andre *et al.*, 2015), and is on the verge of mass production for automotive applications. In addition, the default NMC material in GREET 2018 is switched to $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ (NMC111) from $LiNi_{0.4}Mn_{0.4}Co_{0.2}O_2$ (NMC442), as the former is more common and is available in BatPaC. Additionally, an LIB based on $LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$ (NMC622) is added to GREET 2018, to facilitate future examination of the implications of a switch to Ni-rich cathode chemistries.

The updated BOMs for LIBs based on lithium manganese oxide (LMO), lithium iron phosphate (LFP), NMC111, NMC622, and lithium nickel cobalt aluminum oxide (NCA) are derived from BatPaC version 3.1-28June2018 (ANL, 2018), while the updated BOM for NMC811-based LIB is derived from an internal version of BatPaC. To match the characteristics of EVs in GREET, Battery 1 design in BatPaC is selected for HEV and PHEV batteries, while Battery 5 design is chosen for BEV batteries. The key parameters of chosen batteries are listed in Table 1. The methodology described in Dunn *et al.* (2014) is adopted to compile the LIB BOM based on battery design information in BatPaC. Please note that the 2015 update added two LIBs based on a lithium and manganese-rich metal oxide $0.5Li_2MnO_3 \cdot 0.5LiNi_{0.44}Co_{0.25}Mn_{0.31}O_2$ (LMR-NMC) cathode, coupled with a graphite and silicon anode, respectively (Dunn *et al.*, 2015). Such cathode chemistry no longer exists in BatPaC, so the BOMs of the two LIBs are not updated. Nevertheless, the existing LMR-NMC batteries are retained in GREET 2018, as a potential chemistry for future automotive LIBs.

Table 1. Key Parameters of Chosen EV Batteries

	HEV	PHEV-split	PHEV-series	BEV
Target Pack Power (kW)	100*	100	100	120
Vehicle Range (miles)	N/A	20	40	100
Pack Energy (kWh)	3.6	7.1	14.3	23.5

*Adjusted by 60%, the available battery energy, when calculating specific power for HEV batteries. Such adjustment is not made for PHEV and BEV batteries in the calculation of their specific energy, as available battery energy is already accounted for in GREET in the battery sizing calculation.

Table 2 summarizes the updated specific power for HEV batteries, Table 3 lists the updated specific energy for PHEV and BEV batteries, and Table 4 shows the updated BOMs of all EV battery packs. To enable comparative analysis of our LIB LCA research with other studies, battery BOMs at the cell and module levels are also given in the Appendix. It should be noted that the LIB BOM can vary considerably with cell type, pack configuration, battery size, and desired EV characteristics. The BOMs presented here only represent one specific battery for each EV category. Users of the GREET battery LCA module are therefore encouraged to supply their own LIB BOM if available, or explore BatPaC for a BOM that is more representative of the LIB they are analyzing.

Table 2. Specific Power of HEV Battery Pack

	LMO	NMC111	LFP
Pack Specific Power (W/kg)	2,279	1,995	1,280

Table 3. Specific Energy of PHEV and BEV Battery Pack

	PHEV-split			PHEV-series			BEV					
	LMO	NMC111	LFP	LMO	NMC111	LFP	LMO	NMC111	LFP	NMC622	NMC811	NCA
Pack Specific Energy (Wh/kg)	95.4	113.2	88.9	116.6	140.6	111.5	121.2	142.6	115.9	155.0	149.2	158.6

Table 4. BOMs of EV Battery Packs

	HEV			PHEV-split			PHEV-series			BEV					
	LMO	NMC111	LFP	LMO	NMC111	LFP	LMO	NMC111	LFP	LMO	NMC111	LFP	NMC622	NMC811	NCA
Active Material	17.5%	16.3%	15.5%	24.2%	19.9%	18.1%	29.6%	24.8%	22.8%	30.7%	25.2%	23.8%	23.1%	22.2%	21.6%
Graphite/Carbon	7.3%	10.3%	9.1%	9.9%	12.4%	10.6%	12.1%	15.3%	13.2%	12.7%	15.7%	13.8%	16.5%	15.9%	17.1%
Silicon	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
Binder	1.3%	1.4%	1.3%	1.8%	1.7%	1.5%	2.2%	2.1%	1.9%	2.3%	2.2%	2.0%	2.1%	2.5%	2.0%
Copper	23.8%	23.2%	24.3%	19.5%	21.2%	19.8%	15.2%	16.4%	14.6%	11.6%	11.7%	10.4%	11.8%	11.5%	12.1%
Wrought Aluminum	19.8%	19.5%	20.1%	20.6%	18.2%	20.6%	20.1%	18.7%	20.4%	22.7%	23.9%	23.1%	24.6%	24.5%	24.9%
Cast Aluminum	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
Electrolyte: LiPF6	1.2%	1.3%	1.9%	1.5%	1.4%	2.1%	1.7%	1.7%	2.4%	1.7%	1.6%	2.5%	1.6%	1.8%	1.6%
Electrolyte: Ethylene Carbonate	3.2%	3.5%	5.4%	4.1%	4.0%	5.7%	4.6%	4.6%	6.7%	4.6%	4.5%	6.8%	4.5%	5.1%	4.4%
Electrolyte: Dimethyl Carbonate	3.2%	3.5%	5.4%	4.1%	4.0%	5.7%	4.6%	4.6%	6.7%	4.6%	4.5%	6.8%	4.5%	5.1%	4.4%
Plastic: Polypropylene	1.5%	1.5%	2.0%	1.6%	1.5%	1.4%	1.3%	1.4%	1.2%	1.1%	1.1%	1.0%	1.1%	1.1%	1.1%
Plastic: Polyethylene	0.5%	0.5%	0.5%	0.4%	0.4%	0.4%	0.4%	0.4%	0.3%	0.3%	0.4%	0.3%	0.4%	0.4%	0.4%
Plastic: Polyethylene Terephthalate	0.3%	0.3%	0.3%	0.2%	0.2%	0.2%	0.2%	0.2%	0.2%	0.2%	0.2%	0.2%	0.2%	0.2%	0.2%
Steel	1.2%	1.3%	1.4%	1.0%	1.0%	1.1%	1.0%	1.0%	1.1%	0.6%	0.6%	0.7%	0.6%	0.6%	0.6%
Thermal Insulation	1.0%	0.9%	0.7%	0.5%	0.6%	0.6%	0.4%	0.4%	0.4%	0.4%	0.5%	0.5%	0.5%	0.5%	0.5%
Coolant: Glycol	7.4%	7.0%	5.7%	4.0%	5.1%	5.8%	2.7%	3.5%	4.1%	3.4%	4.3%	5.1%	4.6%	4.6%	4.8%
Electronic Parts	10.9%	9.6%	6.3%	6.7%	8.0%	6.4%	4.1%	5.0%	4.0%	3.1%	3.7%	3.0%	4.0%	3.8%	4.1%

2 CATHODE MATERIALS PRODUCTION

Existing LCIs in GREET 2017 for the production of LCO, NCA, and NMC cathode powders were based on engineering calculations (Dunn *et al.*, 2015, Benavides *et al.*, 2016) and a process model developed at ANL (Dai *et al.*, 2017). Although LCO-based EV LIBs no longer exist in GREET 2018, LCO remains in our repository of cathode materials, to allow for analyses of LIBs beyond automotive applications. In April 2018, with the help of our collaborators at China Automotive Technology and Research Center (CATARC), we visited a leading cathode materials producer in China, and collected material and energy flows data pertaining to their production processes. The collected data serve as the basis for the update of the production of LCO, NCA, and NMC cathode powders in GREET 2018.

2.1 Production of Cathode Materials via Calcination

The plant we visited had an annual production capacity of 27,000 metric ton (t) cathode materials in 2017. Three new production facilities were under construction at the time of our visit. Once completed, the plant will have an annual production capacity of 45,000 t. The plant produces LCO from Co_3O_4 and Li_2CO_3, and NMC from $NMC(OH)_2$ and Li_2CO_3/LiOH, via calcination (a.k.a. solid state synthesis pathway). The production facility we visited has three identical production lines, each with a capacity of 2,000 t of cathode materials per year. At the time of our visit, the facility was being used to produce NMC622 cathode powder. The production process is depicted in Figure 1.

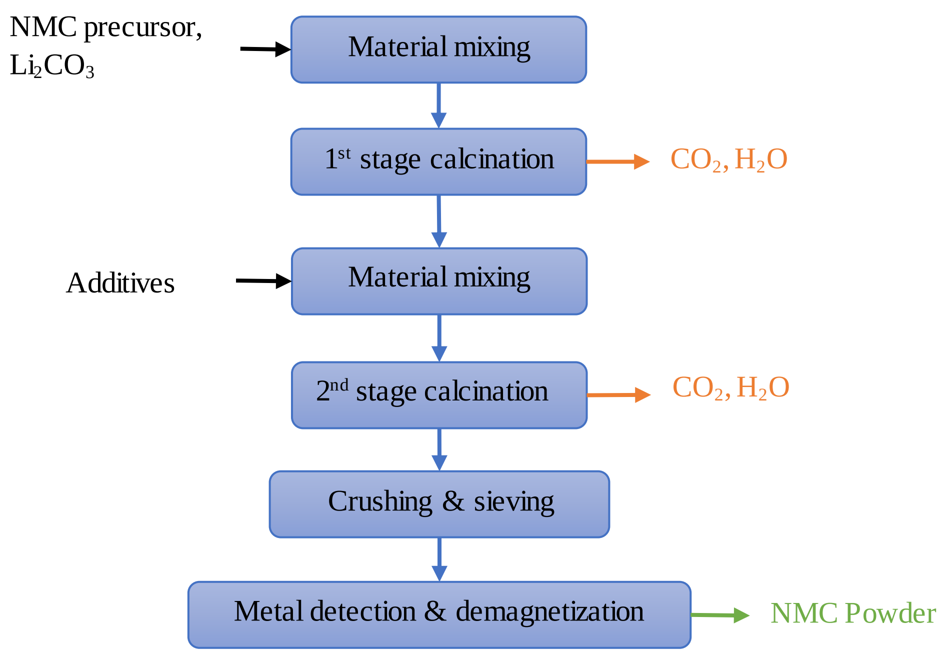

Figure 1. NMC Cathode Powder Production from Precursor via Calcination

The production process is fully automated and is exclusively powered by electricity. Almost all electricity consumption is attributed to the calcination kiln, because the calcination step can last over 12 hours at a temperature over 1000 °C. Compared to the kiln, the electricity consumption by the rest of the equipment is negligible. The entire production process has been designed to minimize material loss. Intermediate materials are transported in tubes between production steps, and the small quantity of dust generated from mixing, crushing, and sieving steps is collected and returned to the feed stream. As a result, the facility can achieve an overall material efficiency that is very close to 100%. As for water consumption, none of the production steps consume water, and all of the water use at the plant is for activities other than material production, such as lawn irrigation, and for use in office buildings and dormitories.

The personnel who oversee the production activities at the plant commented that given the appropriate feed materials, the facility we visited (i.e., the same set of equipment) can be used to produce LCO, NMC of different stoichiometric ratios, and NCA. One major difference in the production process lies in the number of calcination stages required for different cathode materials. Cathode materials for computer, communication, and consumer electronics (3C) applications with a voltage less than 4.3V, such as LCO, only need 1-stage calcination. All cathode materials for traction applications (i.e., NMC and NCA) require 2-stage calcination. Depending on desired material properties, some cathode materials may need 3-stage calcination. Besides the required calcination stages, the preferred lithium source also differs among cathode materials. Typically, Li_2CO_3 is used in the production of LCO, NMC111, and NMC622, while LiOH is used in the production of NMC811 and NCA. In addition, the calcination process for NCA production requires oxygen, while air is sufficient for the production of the rest of the cathode materials.

The personnel also commented that calcination kilns run 24/7 at the plant, as it takes too long for them to reach operating temperature from starting-up. The throughput of a production line consequently dictates the per unit mass electricity demand of the produced cathode materials. The electricity requirement per kg of cathode materials produced also increases with the number of calcination stages required, and Ni-rich materials are the most energy-intensive to produce. If operating at capacity, a production line consumes 6~8 kWh of electricity for each kg of cathode powder produced.

Piecing the information together, we estimate that producing 1 kg of LCO via calcination consumes 6 kWh of electricity, 1kg of Ni-rich cathode material (i.e., NCA and NMC811) consumes 8 kWh, and 1 kg of NMC of other stoichiometric ratios consumes 7 kWh. We also assume that the production process has a material efficiency of 100%. The existing LCI in GREET 2017 for solid state synthesis of LCO already represents calcining Co_3O_4 and Li_2CO_3 with a 100% conversion efficiency. Therefore, no changes are made to the material inputs for this pathway in GREET 2018. However, process CO_2 emissions from thermal decomposition of Li_2CO_3 used in this pathway were not accounted for in GREET 2017, and are estimated based on stoichiometry and added to the solid state LCO LCI in GREET 2018. Also, energy inputs for this pathway are updated to represent the industrial practice. Similarly, energy inputs for NCA production are updated in GREET 2018, while the material inputs remain the same. For NMC materials, both the material inputs and energy inputs are updated in GREET 2018, as the process model used for NMC materials production in GREET 2017 underestimated the material efficiency of the process. The new material inputs, summarized in Table 5 together with all the updated energy inputs and non-combustion process CO_2 emissions, are based on stoichiometric calculations representative of 100% material efficiency.

Table 5. Updated LCIs for Cathode Materials Production via Calcination

	NMC442	NMC111	NMC622	NMC811	NCA	LCO
Material inputs (ton/ton product)						
Precursor	0.949	0.949	0.949	0.949	N/A	N/A
Li_2CO_3	0.384	0.383	0.381	---	N/A	N/A
LiOH	---	---	---	0.246	N/A	N/A
Energy consumption (mmBtu/ton product)						
Electricity	21.670	21.670	21.670	24.765	24.765	18.574
Non-combustion process emissions (g/ton product)						
CO_2	207,562	206,956	205,956	---	N/A	203,974

2.2 Production of NMC and NCA Precursors

Although the plant we visited does not produce NMC and NCA precursors, another plant owned by the battery producer does, and the materials and energy flows for the production process were disclosed in an environmental protection inspection and monitoring report submitted by the company (Shanshan, 2018).

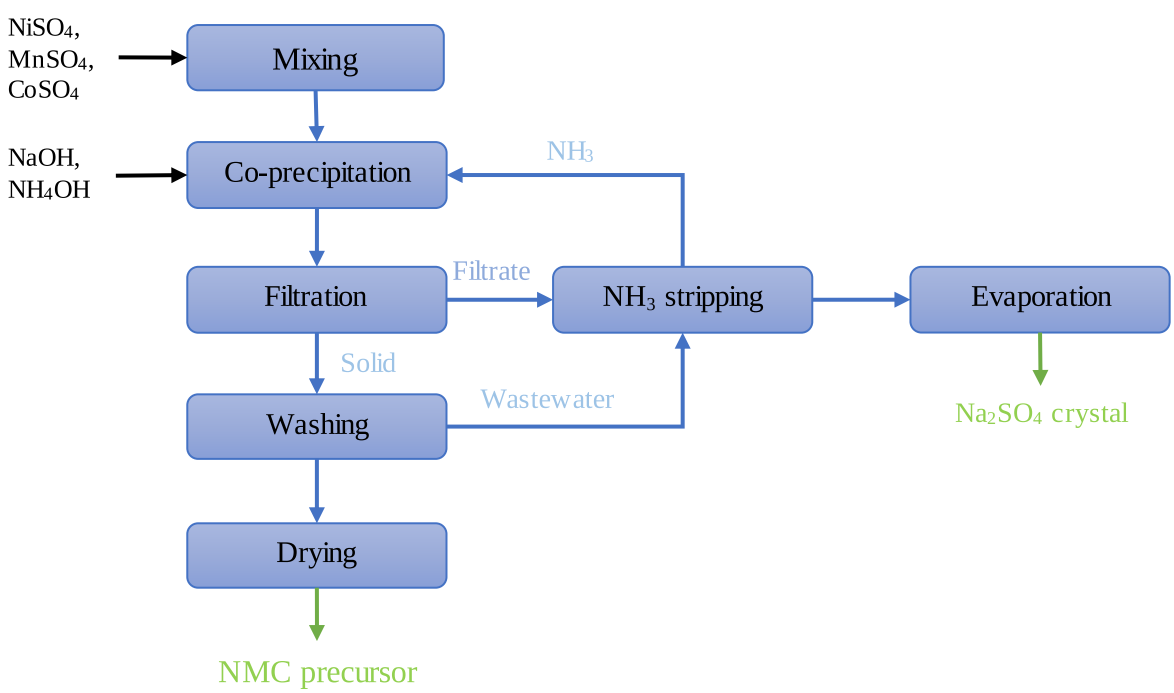

Figure 2. NMC Precursor Production via Co-precipitation

The NMC precursor production process is depicted in Figure 2. It begins with dissolving and mixing stoichiometric ratio of nickel sulfate ($NiSO_4$), manganese sulfate ($MnSO_4$), and cobalt sulfate ($CoSO_4$) in a tank reactor. Once completely dissolved and mixed, sodium hydroxide (NaOH) and ammonium hydroxide (NH_4OH) are added to the solution. The reactor is then heated by steam to 50 °C and kept warm for a prolonged period of time, at the end of which Ni, Mn, and Co co-precipitate out as $NMC(OH)_2$. The $NMC(OH)_2$ solid is then filtered out, washed, and dried to produce the NMC precursor. Na_2SO_4 crystal is a byproduct of the process, produced by feeding the filtrate to a four-effect evaporator. In the presence of slightly excessive amounts of the alkaline reagents, Ni, Mn, and Co reportedly have a conversion efficiency of ~100%. The excess ammonia is removed from the wastewater in an ammonia stripping tower, and is recycled for subsequent precursor production (Shanshan, 2018).

The process consumes 13.37 t of steam per t of precursor produced. Steam is used for alkali pretreatment, reactor heating, ammonia stripping, and evaporation, with a maximum consumption rate of 9.2, 10.5, 6.0, and 9.9 t/hr, respectively (Shanshan, 2018). The steam is supplied by a neighboring power plant, and the temperature of the steam is 200 °C (Dawukou, 2018). Electricity consumption for the precursor production process is not stated in the report. Since none of the equipment listed in the report for precursor production would consume considerable amounts of electricity, and another leading NMC precursor producer reported that the electricity consumption of the co-precipitation step is negligible (Xie *et al.*, 2015), it is assumed that the precursor production process is 100% powered by steam. In terms of water consumption, the plant withdrawals 1,607m^3 of water per day. However, the water balance of the plant shows that the production process only consumes water via evaporative loss, which is estimated to be 0.7t/t precursor produced (Shanshan, 2018).

Table 6. Materials and Energy Flows for NMC532 Precursor Production

	Quantity	Unit
Material inputs		
$NiSO_4.6H_2O$	1.475	ton/ton
$CoSO_4.7H_2O$	0.635	ton/ton
$MnSO_4.H_2O$	0.553	ton/ton
NaOH (48%)	1.853	ton/ton
NH_4OH (20% as NH_3)	0.3	ton/ton
Water consumption		
Water	0.7	ton/ton
Energy consumption		
Steam	13.37	ton/ton

The materials and energy flows for NMC532 precursor production are listed in Table 6. Since the existing LCIs for NMC precursors production in GREET 2017 were based on a process model (Dai *et al.*, 2017), which underestimated material efficiency and did not consider water reuse and wastewater treatment, they are updated based on the new industry data. The same NaOH, NH_4OH, water and steam requirements are assumed for the production of all NMC precursors of different stoichiometric ratios, while the $NiSO_4$, $MnSO_4$, and $CoSO_4$ demands are calculated based on stoichiometry, assuming 100% material efficiency. The steam use is converted into natural gas consumption as follows for GREET implementation:

$$Natural\ gas\ use = \frac{h_{g@200℃} - h_{f@25℃}}{\eta_{boiler}} = \frac{2792kJ/kg - 104.83kJ/kg}{0.8} = \frac{3359kJ}{kg\ steam}$$

Where h_g is the specific enthalpy of saturated water vapor, h_f is the specific enthalpy of saturated water liquid, and η_{boiler} is the boiler efficiency.

Since the NMC precursor production process described above can also be used to produce the NCA precursor, the industry data is also used to update the existing LCI in GREET 2017 for NCA precursor production. As noted before, the existing material inputs in GREET for NCA precursor production already represent the industrial practice, so only the water consumption and energy use are updated in GREET 2018. All the updates of material inputs, water consumption, and energy use for the production of NMC and NCA precursors are summarized in Table 7. It should be noted that all materials and energy consumptions for the production process are ascribed to the precursor on the premise of the Na_2SO_4 crystal being a byproduct. Admittedly, the production of Na_2SO_4 crystal by evaporation consumes energy. However, this process step can also be interpreted as sodium and sulfate removal and thus constitutes wastewater treatment. For this reason, the steam consumption by the evaporator is also attributed to precursor production.

Table 7. Updated LCIs for NMC and NCA Precursors Production

	NMC442	NMC111	NMC622	NMC811	NCA
Material inputs (ton/ton product)					
$NiSO_4$	0.678	0.564	1.009	1.340	N/A
$CoSO_4$	0.340	0.564	0.337	0.168	N/A
$MnSO_4$	0.662	0.550	0.328	0.163	N/A
NaOH (100%)	0.890	0.890	0.890	0.890	N/A
NH_4OH (100%)	0.124	0.124	0.124	0.124	N/A
Water consumption (gal/ton product)					
Water	168.62	168.62	168.62	168.62	168.62
Energy consumption (mmBtu/ton product)					
Natural gas	38.618	38.618	38.618	38.618	38.618

Appendix: BOMs of EV Battery Cells, Modules, and Packs

Table 8. BOMs of EV Battery Cells, Modules and Packs

	HEV			PHEV-split			PHEV-series			BEV					
	LMO	NMC 111	LFP	LMO	NMC 111	LFP	LMO	NMC 111	LFP	LFP	LMO	NCA	NMC 111	NMC 622	NMC 811
Cell components (kg)															
Active cathode material	4.60	4.89	7.27	18.09	12.58	14.57	36.21	25.19	29.22	48.21	59.67	32.11	41.52	35.01	34.93
Graphite	1.61	2.75	3.76	6.22	7.00	7.49	12.35	13.90	14.92	24.85	20.56	23.18	23.18	22.73	23.15
Carbon black	0.31	0.33	0.49	1.22	0.85	0.98	2.44	1.70	1.97	3.25	4.02	2.16	2.80	2.36	1.94
Binder (PVDF)	0.34	0.42	0.61	1.34	1.08	1.21	2.68	2.15	2.43	4.02	4.43	3.02	3.55	3.16	4.01
Copper	3.85	4.51	8.59	10.96	9.33	10.93	15.11	12.85	13.93	20.51	21.99	17.49	18.84	17.37	17.65
Aluminum	1.98	2.33	4.44	5.57	4.73	5.68	7.98	6.76	7.65	11.13	11.47	9.04	9.80	9.03	9.25
Electrolyte: LiPF6	0.30	0.38	0.91	1.10	0.92	1.65	2.02	1.68	3.09	4.98	3.20	2.37	2.66	2.43	2.89
Electrolyte: Ethylene Carbonate	0.85	1.05	2.55	3.07	2.56	4.60	5.65	4.68	8.61	13.89	8.94	6.60	7.43	6.79	8.07
Electrolyte: Dimethyl Carbonate	0.85	1.05	2.55	3.07	2.56	4.60	5.65	4.68	8.61	13.89	8.94	6.60	7.43	6.79	8.07
Plastic: Polypropylene	0.39	0.46	0.93	1.16	0.98	1.15	1.63	1.37	1.48	1.97	2.16	1.68	1.82	1.66	1.68
Plastic: Polyethylene	0.09	0.11	0.22	0.27	0.23	0.27	0.38	0.32	0.34	0.44	0.50	0.39	0.42	0.38	0.39
Plastic: Polyethylene Terephthalate	0.07	0.08	0.13	0.16	0.13	0.18	0.26	0.22	0.29	0.45	0.39	0.31	0.34	0.32	0.34
Subtotal: Cell	15.25	18.37	32.44	52.25	42.94	53.32	92.36	75.49	92.55	147.58	146.29	104.96	119.77	108.03	112.37
Module components sans cell (kg)															
Copper	0.20	0.21	0.23	0.18	0.20	0.25	0.18	0.20	0.23	0.51	0.39	0.43	0.43	0.43	0.44
Aluminum	0.86	0.98	1.56	2.88	2.50	3.25	4.56	3.92	5.16	9.39	8.27	6.64	7.22	6.77	7.15
Plastic: Polyethylene	0.04	0.04	0.04	0.05	0.05	0.05	0.05	0.05	0.05	0.18	0.18	0.18	0.18	0.18	0.18
Insulation	0.05	0.05	0.06	0.04	0.05	0.06	0.04	0.05	0.06	0.13	0.10	0.11	0.11	0.11	0.11
Electronic part	0.42	0.42	0.42	0.42	0.42	0.42	0.42	0.42	0.42	1.12	1.12	1.12	1.12	1.12	1.12
Subtotal: Module sans cell	1.56	1.69	2.31	3.57	3.22	4.03	5.25	4.63	5.92	11.32	10.05	8.47	9.06	8.60	9.00
Pack components sans module (kg)															
Copper	2.21	2.26	2.56	3.43	3.88	4.75	3.28	3.66	4.50	0.11	0.08	0.09	0.09	0.09	0.09
Aluminum	2.37	2.56	3.42	6.95	4.25	7.58	12.11	8.28	13.31	26.34	24.25	21.31	22.33	21.50	22.29
Steel	0.33	0.38	0.67	0.71	0.62	0.85	1.21	1.02	1.42	1.44	1.19	0.92	1.02	0.94	1.01
Insulation	0.21	0.23	0.28	0.34	0.32	0.39	0.42	0.40	0.48	0.82	0.75	0.66	0.69	0.67	0.69
Coolant	1.95	2.12	2.69	3.02	3.24	4.65	3.30	3.51	5.26	10.35	6.62	7.07	7.10	7.02	7.30
Electronic part	2.45	2.46	2.52	4.60	4.66	4.76	4.60	4.64	4.72	5.03	4.84	4.91	4.91	4.90	4.93
Subtotal: Pack sans module	9.51	10.01	12.14	19.05	16.96	22.98	24.92	21.52	29.68	44.09	37.73	34.95	36.15	35.12	36.32
Total: Pack	26.32	30.07	46.89	74.86	63.13	80.33	122.53	101.64	128.15	202.99	194.07	148.38	164.98	151.76	157.68

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