# Update of Bill-of-Materials and Cathode Chemistry addition for Lithium-ion Batteries in GREET® 2020

by

O. Winjobi, Q. Dai, and J.C. Kelly

Systems Assessment Group

Energy Systems Division

Argonne National Laboratory

October 2020

## CONTENTS



## TABLES

# ACRONYMS

| | |
|---|---|
| BatPaC | Battery Performance and Cost |
| BEV | battery electric vehicle |
| BOM | bill-of-material |
| | |
| EV | electric vehicle |
| | |
| HEV | hybrid electric |
| | |
| 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 electric vehicle |

*This page intentionally left blank.*

# Update of Bill-of-Material and Cathode Chemistry addition for Lithium-ion Batteries in GREET® 2020


Olumide Winjobi, Qiang Dai, and Jarod C. Kelly

Systems Assessment Group

Energy Systems Division

Argonne National Laboratory


October 2020


This memo documents updates in the GREET® model for 1) bill-of-materials (BOM) of lithium-ion batteries (LIBs) for electric vehicles (EVs), including hybrid electric vehicles (HEVs), plug-in hybrid electric vehicles (PHEVs), and battery electric vehicles (BEVs); 2) the life cycle inventory (LCI) for the production of an added lithium nickel cobalt manganese oxide (NMC) cathode chemistry, $LiNi_{0.5}Mn_{0.3}Co_{0.2}$ (NMC532). The BOM update was based on the most recent version of Argonne's Battery Performance and Cost (BatPaC) model (version 4.0). The NMC532 update was adapted from existing LCIs in GREET for other NMC chemistries.


## 1. Introduction

Existing BOMs for LIBs in GREET 2019 were last updated in 2018, based on BatPaC version 3.0 (Dai et al., 2018). However, a new version of BatPaC, version 4.0, was released in 2020 with updates to the BOM, power, and energy characteristics associated with LIB of varying cathode chemistries. The LIB characteristics are therefore updated in GREET 2020 to account for these changes. NMC532, a cathode chemistry that accounts for a significant portion of the current LIB market share is also added to the cathode chemistry for BEVs in GREET2020.

## 2. Updated Specific Energy and Bill-of-Materials

The updated BOMs for LIBs based on seven cathode chemistries, including $LiMn_2O_4$ (LMO), $LiFePO_4$ (LFP), $LiNi_{0.3}Mn_{0.3}Co_{0.3}O_2$ (NMC111), $LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$ (NMC622), $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC811), $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (NCA), and the newly added NMC532, are derived from BatPaC version 4.0. For the BOM update in GREET, the 'Battery 1" design in

BatPaC 4.0 is selected for HEV and PHEV batteries, while the “Battery 5” design is chosen for BEV batteries. The key parameters of the chosen batteries are listed in Table 1. The methodology described in previous work is adopted to compile the LIB BOM based on battery design information in BatPaC 4.0 (Dunn et al., 2014, Dai et al., 2018). A vehicle range of 300 miles was set in BatPaC 4.0 for BEVs to reflect the current push for longer range BEVs.

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 | 300 |
| Pack Energy (kWh) | 2.8 | 7.1 | 14.3 | 70.6 |

*Adjusted by utilizing 60% of the available battery energy, when calculating the specific power for HEV batteries.

Adapting the work of Dai et al. (2018), in calculating the specific power for HEV batteries in GREET, the available battery energy is adjusted by utilizing 60% of the specific power calculated from BatPaC in GREET. The adjustment is not carried out for PHEV and BEV batteries because the available battery energy for PHEV and BEV is already accounted for in GREET in their battery sizing calculation. Table 2 summarizes the updated specific power for HEV batteries, while Table 3 lists the updated specific energy for PHEV and BEV batteries.

Table 2. Specific Power of HEV Battery Pack

| | LMO | NMC111 | LFP |
|---|---|---|---|
| Pack Specific Power (W/kg) | 2,276 | 2,337 | 1,584 |

To enable comparative analysis of our LIB LCA with other studies, battery BOMs at the cell and module levels are also provided in the Appendix. It is worth noting 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 3. Specific Energy of PHEV and BEV Battery Pack

| | PHEV-split | | | PHEV-series | | | BEV | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | LMO | NMC111 | LFP | LMO | NMC111 | LFP | LMO | NMC111 | LFP | NMC532 | NMC622 | NMC811 | NCA |
| Pack Specific Energy (Wh/kg) | 146.5 | 155.1 | 107.1 | 153.7 | 173.7 | 128.0 | 184.4 | 214.8 | 174.1 | 224.7 | 240.7 | 247.9 | 250.9 |

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 | NMC532 | NMC622 | NMC811 | NCA |
| Active Material | 24.71% | 19.05% | 14.92% | 34.45% | 27.38% | 21.85% | 36.19% | 30.81% | 26.24% | 43.46% | 38.17% | 35.96% | 38.56% | 36.10% | 31.54% | 34.58% |
| Carbon | 8.94% | 10.15% | 7.96% | 12.38% | 14.49% | 11.62% | 12.97% | 16.28% | 13.93% | 15.58% | 20.17% | 19.11% | 20.57% | 22.07% | 24.44% | 23.42% |
| Silicon | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% |
| Binder | 0.69% | 0.91% | 0.47% | 0.96% | 1.30% | 0.68% | 1.00% | 1.47% | 0.82% | 1.20% | 1.81% | 1.12% | 1.21% | 1.19% | 2.22% | 1.18% |
| Copper | 15.16% | 17.61% | 23.86% | 9.82% | 12.26% | 16.95% | 11.26% | 11.52% | 13.88% | 8.23% | 7.21% | 8.26% | 7.16% | 7.08% | 7.23% | 6.82% |
| Wrought Aluminum | 17.12% | 18.19% | 20.49% | 14.88% | 16.06% | 20.35% | 16.10% | 16.09% | 19.54% | 16.83% | 17.26% | 17.52% | 17.33% | 17.85% | 18.41% | 18.00% |
| Cast Aluminum | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% | 0.00% |
| LiPF6 | 1.43% | 1.40% | 1.75% | 1.71% | 1.68% | 2.06% | 1.75% | 1.72% | 2.19% | 1.39% | 1.38% | 1.78% | 1.31% | 1.37% | 1.39% | 1.36% |
| Ethylene Carbonate | 3.98% | 3.90% | 4.88% | 4.77% | 4.69% | 5.75% | 4.90% | 4.79% | 6.11% | 3.87% | 3.87% | 4.98% | 3.67% | 3.81% | 3.88% | 3.80% |
| Dimethyl Carbonate | 3.98% | 3.90% | 4.88% | 4.77% | 4.69% | 5.75% | 4.90% | 4.79% | 6.11% | 3.87% | 3.87% | 4.98% | 3.67% | 3.81% | 3.88% | 3.80% |
| Polypropylene | 1.40% | 1.67% | 2.49% | 0.88% | 1.14% | 1.75% | 0.78% | 0.64% | 1.05% | 0.79% | 0.66% | 0.80% | 0.79% | 0.63% | 0.76% | 0.60% |
| Polyethylene | 0.38% | 0.45% | 0.63% | 0.24% | 0.30% | 0.44% | 0.20% | 0.17% | 0.27% | 0.21% | 0.18% | 0.21% | 0.22% | 0.18% | 0.22% | 0.18% |
| Polyethylene Terephthalate | 0.25% | 0.25% | 0.26% | 0.21% | 0.21% | 0.22% | 0.21% | 0.21% | 0.22% | 0.18% | 0.19% | 0.20% | 0.18% | 0.19% | 0.20% | 0.19% |
| Steel | 2.37% | 2.36% | 2.59% | 1.97% | 1.97% | 2.08% | 1.28% | 1.27% | 1.38% | 0.58% | 0.60% | 0.67% | 0.58% | 0.60% | 0.62% | 0.60% |
| Thermal Insulation | 0.80% | 0.84% | 0.66% | 0.52% | 0.58% | 0.54% | 0.50% | 0.61% | 0.59% | 0.30% | 0.33% | 0.32% | 0.34% | 0.36% | 0.37% | 0.37% |
| Coolant: Glycol | 3.90% | 3.97% | 3.52% | 3.87% | 4.04% | 3.58% | 3.50% | 4.49% | 3.90% | 2.07% | 2.61% | 2.70% | 2.71% | 2.95% | 2.97% | 3.19% |
| Electronic Parts | 14.89% | 15.36% | 10.63% | 8.59% | 9.21% | 6.39% | 4.46% | 5.15% | 3.78% | 1.43% | 1.69% | 1.39% | 1.70% | 1.82% | 1.88% | 1.90% |

# 3. NMC532 Cathode Material Production

Existing LCIs in GREET 2019 for the production of NMCs are based on our site visit to one leading cathode material producer, literature, and industry reports, as described by Dai et al. (2018) The LCI for the production of the NMC532 cathode was adapted from the existing LCI in GREET for other NMC chemistries.

## 3.1 Production of NMC532 Cathode Materials via Calcination

The methodology used by Dai et al. (2018) was adopted for the production of NMC532 via calcination. 1kg of NMC532 consumes 7kWh of electricity and has an assumed material efficiency of 100%. The material and energy inputs for the production are shown in Table 5. The material inputs and non-combustion process $CO_2$ emissions are based on stoichiometric calculations assuming 100% efficiency.

Table 5. LCI for NMC532 Cathode Material Production via Calcination

| | |
|---|---|
| **Material inputs (ton/ton product)** | |
| NMC532 Precursor | 0.945 |
| $Li_2CO_3$ | 0.381 |
| **Energy consumption (mmBtu/ton product)** | |
| Electricity | 21.670 |
| **Non-combustion process emissions (g/ton product)** | |
| $CO_2$ | 205,895 |

## 3.2 Production of NMC532 Precursor

The production of the NMC532 precursor uses a co-precipitation process as described by Dai et al (2018). The materials and energy requirements for NMC532 production are based on industry data reported by Dai et al. (2018), as summarized in Table 6.

The steam requirement is converted into natural gas consumption 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 $\eta_{boiler}$ is the boiler efficiency.

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 LCI for NMC532 precursor production to be incorporated into GREET2020 are shown in Table 7.

Table 7. LCI for NMC532 Precursor Production

| | |
|---|---|
| **Material inputs (ton/ton product)** | |
| $NiSO_4$ | 0.868 |
| $CoSO_4$ | 0.350 |
| $MnSO_4$ | 0.494 |
| NaOH (100%) | 0.890 |
| $NH_4OH$ (100%) | 0.124 |
| **Water consumption (gal/ton product)** | |
| Water | 168.62 |
| **Energy consumption (mmBtu/ton product)** | |
| Natural gas | 38.618 |

# APPENDIX

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

| | HEV | | | PHEV-split | | | PHEV-series | | | BEV | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | LMO | NMC 111 | LFP | LMO | NMC 111 | LFP | LMO | NMC 111 | LFP | LMO | NMC 111 | LFP | NMC 532 | NMC 622 | NMC 811 | NCA |
| Active cathode material | 6.52 | 4.89 | 5.65 | 16.80 | 12.61 | 14.57 | 33.63 | 25.34 | 29.28 | 166.35 | 125.43 | 145.78 | 121.11 | 105.87 | 89.81 | 97.27 |
| Carbon black | 0.14 | 0.10 | 0.12 | 0.35 | 0.26 | 0.30 | 0.70 | 0.53 | 0.61 | 3.47 | 2.61 | 3.04 | 2.52 | 2.21 | 4.99 | 2.03 |
| Graphite | 2.22 | 2.50 | 2.90 | 5.69 | 6.41 | 7.44 | 11.36 | 12.86 | 14.93 | 56.19 | 63.67 | 74.44 | 62.07 | 62.52 | 64.60 | 63.87 |
| Binder (PVDF) | 0.18 | 0.23 | 0.18 | 0.47 | 0.60 | 0.46 | 0.93 | 1.20 | 0.91 | 4.61 | 5.96 | 4.56 | 3.79 | 3.48 | 6.31 | 3.33 |
| Copper | 3.57 | 4.08 | 8.55 | 4.34 | 5.15 | 10.77 | 7.26 | 5.52 | 11.25 | 31.02 | 23.17 | 32.90 | 21.97 | 20.25 | 20.06 | 18.67 |
| Aluminum | 1.88 | 2.09 | 4.27 | 2.41 | 2.74 | 5.48 | 4.15 | 3.25 | 6.19 | 17.00 | 13.13 | 18.50 | 12.38 | 11.50 | 11.45 | 10.70 |
| Electrolyte: LiPF6 | 0.38 | 0.36 | 0.66 | 0.83 | 0.77 | 1.37 | 1.63 | 1.41 | 2.44 | 5.30 | 4.55 | 7.23 | 4.13 | 4.01 | 3.96 | 3.83 |
| Electrolyte: Ethylene Carbonate | 1.05 | 1.00 | 1.85 | 2.33 | 2.16 | 3.83 | 4.55 | 3.94 | 6.82 | 14.80 | 12.70 | 20.19 | 11.53 | 11.19 | 11.05 | 10.70 |
| Electrolyte: Dimethyl Carbonate | 1.05 | 1.00 | 1.85 | 2.33 | 2.16 | 3.83 | 4.55 | 3.94 | 6.82 | 14.80 | 12.70 | 20.19 | 11.53 | 11.19 | 11.05 | 10.70 |
| Plastic: Polypropylene | 0.37 | 0.43 | 0.95 | 0.43 | 0.53 | 1.17 | 0.72 | 0.52 | 1.18 | 3.04 | 2.17 | 3.23 | 2.48 | 1.85 | 2.18 | 1.68 |
| Plastic: Polyethylene | 0.09 | 0.10 | 0.23 | 0.10 | 0.12 | 0.28 | 0.16 | 0.11 | 0.27 | 0.68 | 0.47 | 0.72 | 0.56 | 0.40 | 0.48 | 0.36 |
| Plastic: Polyethylene Terephthalate | 0.07 | 0.06 | 0.10 | 0.10 | 0.10 | 0.14 | 0.19 | 0.17 | 0.24 | 0.70 | 0.62 | 0.82 | 0.58 | 0.55 | 0.56 | 0.53 |
| Subtotal: Cell | 17.50 | 16.86 | 27.29 | 36.16 | 33.60 | 49.64 | 69.84 | 58.79 | 80.96 | 317.95 | 267.21 | 331.57 | 254.63 | 235.02 | 226.49 | 223.67 |
| Module components sans cell (kg) | | | | | | | | | | | | | | | | |
| Copper | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.25 | 0.30 | 0.32 | 0.39 | 0.43 | 0.48 | 0.42 | 0.43 | 0.43 | 0.43 |
| Aluminum | 0.76 | 0.74 | 1.10 | 1.86 | 1.77 | 2.55 | 3.53 | 3.12 | 4.38 | 13.94 | 12.48 | 16.13 | 11.76 | 11.32 | 11.42 | 10.94 |
| Plastic: Polyethylene | 0.01 | 0.01 | 0.01 | 0.02 | 0.02 | 0.02 | 0.03 | 0.03 | 0.03 | 0.13 | 0.13 | 0.13 | 0.13 | 0.13 | 0.13 | 0.13 |
| Insulation | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.06 | 0.07 | 0.08 | 0.10 | 0.11 | 0.12 | 0.11 | 0.11 | 0.11 | 0.11 |
| Electronic part | 0.21 | 0.21 | 0.21 | 0.21 | 0.21 | 0.21 | 0.32 | 0.32 | 0.32 | 1.12 | 1.12 | 1.12 | 1.12 | 1.12 | 1.12 | 1.12 |
| Subtotal: Module sans cell | 0.98 | 0.96 | 1.32 | 2.09 | 1.99 | 2.78 | 4.19 | 3.85 | 5.13 | 15.68 | 14.27 | 17.99 | 13.54 | 13.10 | 13.20 | 12.74 |
| Pack components sans module (kg) | | | | | | | | | | | | | | | | |
| Copper | 0.43 | 0.44 | 0.49 | 0.45 | 0.49 | 0.53 | 0.26 | 0.32 | 0.35 | 0.08 | 0.09 | 0.10 | 0.09 | 0.09 | 0.09 | 0.09 |
| Aluminum | 1.87 | 1.84 | 2.40 | 2.99 | 2.89 | 5.53 | 7.28 | 6.85 | 11.23 | 33.48 | 31.09 | 36.37 | 30.31 | 29.52 | 29.56 | 29.00 |
| Steel | 0.63 | 0.60 | 0.98 | 0.96 | 0.91 | 1.39 | 1.19 | 1.05 | 1.54 | 2.23 | 1.98 | 2.71 | 1.83 | 1.76 | 1.78 | 1.69 |
| Insulation | 0.21 | 0.22 | 0.25 | 0.25 | 0.27 | 0.36 | 0.40 | 0.43 | 0.58 | 1.06 | 0.99 | 1.16 | 0.97 | 0.94 | 0.94 | 0.93 |
| Coolant | 1.03 | 1.02 | 1.34 | 1.89 | 1.86 | 2.38 | 3.25 | 3.70 | 4.35 | 7.92 | 8.58 | 10.94 | 8.50 | 8.65 | 8.47 | 8.97 |
| Electronic part | 3.72 | 3.74 | 3.82 | 3.98 | 4.03 | 4.05 | 6.52 | 7.26 | 7.46 | 4.36 | 4.43 | 4.50 | 4.22 | 4.22 | 4.22 | 4.23 |
| Subtotal: Pack sans module | 7.89 | 7.86 | 9.28 | 10.52 | 10.45 | 14.25 | 18.90 | 19.60 | 25.50 | 49.14 | 47.16 | 55.79 | 45.91 | 45.18 | 45.06 | 44.90 |
| **Total: Pack** | **26.37** | **25.68** | **37.89** | **48.77** | **46.04** | **66.67** | **92.93** | **82.24** | **111.59** | **382.77** | **328.64** | **405.35** | **314.09** | **293.30** | **284.75** | **281.31** |

# REFERENCES


ANL, 2020. BatPaC: A Lithium-Ion Battery Performance and Cost Model for Electric-Drive Vehicles: http://www.cse.anl.gov/batpac/

Dai, Q., J. C. Kelly, J. Dunn, and P. T. Benavides. "Update of bill-of-materials and cathode materials production for lithium-ion batteries in the GREET model." *Argonne National Laboratory* (2018). https://greet.es.anl.gov/publication-update_bom_cm

Dunn, J., Gaines, L., Barnes, M., Sullivan, J., and Wang, M. *Material and energy flows in the materials production, assembly, and end-of-life stages of the automotive lithium-ion battery life cycle*. No. ANL/ESD/12-3 Rev. Argonne National Lab. (ANL), Argonne, IL (United States), 2014. https://greet.es.anl.gov/publication-li-ion