Clean Technologies and Recycling

http://www.aimspress.com/journal/ctr

Clean Technologies and Recycling, 1(1): 34–49.
DOI: 10.3934/ctr.2021002
Received: 23 February 2021
Accepted: 01 June 2021
Published: 30 June 2021

Research article

A market-oriented database design for critical material research

Ruby T. Nguyen[1,*], Ange-Lionel Toba[1], Michael H. Severson[1], Ethan M. Woodbury[2], Austin R. Carey[3] and D. Devin Imholte[1]

[1] Idaho National Laboratory, Idaho Falls, ID 83415, USA
[2] UC Berkeley, Berkeley, CA 94720, USA
[3] Brigham Young University–Idaho, Rexburg, ID 83460, USA

* **Correspondence:** Email: ruby.nguyen@inl.gov.

Supplementary

Methodology for quantifying elemental content in vehicle batteries

Considering top vehicle models occupied at least 80% of total sold vehicles between 2000 and 2017 for each category, Nissan Leaf, Tesla Model S, Tesla Model X, BMW i3 and Chevy Bolt occupied 86% of total sold BEVs while Toyota Prius Plug-in, Chevy Volt, Ford Fusion Energi and Ford C-Max Energi accounted for 91% of sold PHEVs. Ten hybrid models occupying 81% sold HEVs include Toyota Prius hybrid, Toyota Camry hybrid, Honda Civic hybrid, Ford Fusion hybrid, Lexus RX 400h/450h, Toyota Prius C, Toyota Highlander hybrid, Toyota Prius V, Ford Escape hybrid and Hyundai Sonata hybrid.

Quantifying battery material content

The material within each vehicle model's battery pack was calculated by considering the cell chemistry, cell capacity (Ah), and number of cells. Battery information was collected from online datasheets by vehicle manufacturers, news articles, and previously published academic papers and reports on EVs. Previous methods obtained material content from the Bat Pac model (Argonne National Laboratory n.d.-a), using battery capacity and size (Tahil 2010) or voltage and size (Speirs et al. 2014). Of these three methods, the Bat Pac model is the most comprehensive by applying a bottom up approach to calculate material content, total cost of manufacturing and recycling value of battery metals (Argonne National Laboratory n.d.-a). In this paper, we utilize a subset of equations from the Bat Pac model. The first step was to calculate the theoretical mass of the cell's cathode to derive Li and Co masses. Since Li is also present in the electrolyte, an additional calculation step was needed. The electrolyte requirement, electrolyte concentration, and electrolyte density values are typical values for lithium ion batteries and were assumed to be constant across battery chemistries. Equations (1) through (4) illustrate calculation steps. Specific capacities used in calculations are shown in Table S1.

$$m_{Co} = \frac{n_{cells}}{1000} \cdot \left(\frac{1000 * a_{cells}}{s_{cat}} \cdot \frac{x_{Co} M_{Co}}{M_{cat}}\right) \text{ (Eq 1)}$$

where:

m_{Co} is the mass of Co in a battery pack in g
n_{cells} is the number of cells in the battery pack
a_{cells} is the cell capacity in Ah
s_{cat} is the specific capacity of the cathode chemistry in mAh/g
x_{Co} is the stoichiometric coefficient of cobalt in the cathode formula
M_{Co} is the molar mass of cobalt (58.933 g/mol)
M_{cat} is the molar mass of the cathode compound

$$m_{Li,cat} = \frac{1000 * a_{cell}}{s_{cat}} \cdot \frac{M_{Li}}{M_{cat}} \text{ (Eq 2)}$$

where:

$m_{Li,cat}$ is the mass of Li in cathode of a cell in g
a_{cell} is the cell's capacity in Ah
s_{cat} is the theoretical specific capacity of the cathode chemistry in mAh/g
M_{Li} is the Li molar mass (6.941 g/mol)
M_{cat} is the cathode compound's molar mass

$$m_{Li,elec} = \frac{a_{cell} e_{elec} c_{elec} M_{Li}}{1000 * \rho_{elec}} \text{ (Eq 3)}$$

where:

$m_{Li,elec}$ is the mass of Li in the electrolyte of a cell in g
a_{cell} is the cell's capacity in Ah
e_{elec} is the electrolyte requirement (1.2g/Ah)
c_{elec} is the electrolyte concentration (1.1M $LiPF_6$)
M_{Li} is the molar mass of Li
ρ_{elec} is the density of the electrolyte (1.3g/mL)

$$m_{Li,pack} = \frac{n_{cells}}{1000} \cdot (m_{Li,cat} + m_{Li,elec}) \text{ (Eq 4)}$$

Table S1. Specific capacities for cathode chemistries used in Equation (1) and (2), calculated by Faraday's law

Cathode chemistry	Theoretical specific capacity (mAh/g)
NMC-LMO	151
NCA	190
LFP	170
LMO	110

Although this approach accounts for individual cell chemistry, it had several limitations. First, NMC-LMO chemistry varies greatly among cell manufacturers, with manufacturers using a range of stoichiometric ratios between 25% NMC: 75% LMO up to 100% NMC. Over time, manufacturers have been shifting toward higher NMC blends because of NMC's superior capacity, but blends by specific manufacturers are proprietary information. In this paper, we assumed every NMC-LMO cell has a ratio of 75% NMC: 25% LMO, which appears to be a common choice among manufacturers. The Li and Co content in LMO-NMC blended cells were calculated using a weighted average of materials required if the cells instead had been pure LMO and pure NMC.

As discussed previously, NMC chemistries have also been changing over time, with manufacturers switching to blends with higher nickel content such as NMC 523, 622, and 811 to increase capacity and decrease costs due to cobalt. This information is also proprietary. For the purpose of this analysis, we assumed that manufacturers used NMC 111 before 2016 and switched to NMC 523 for the 2016 model year.

Other assumptions were that polymer electrolytes contain the same Li content as organic electrolytes. If the number of cells and cell capacity were not available, we assumed a typical battery configuration, cell size, and number of cells consistent with the total kWh rating of the car. We also assumed that battery cathodes have the exact same capacity as their theoretical capacity, when in reality the actual capacity is somewhat lower.