

## Supporting Information

### **Towards More Environmentally and Socially Responsible Batteries**

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# Battery Cell Modeling

Generally speaking, the components of a battery include: a cathode, anode, electrolyte, separator, conductive additives, binder, current collectors, and cell casing. In addition, solvents (typically NMP or water) are used to prepare electrode slurries. For this article, a pouch cell form factor with a double-sided cathode, two single-sided anodes, and four layers of separator was assumed. Since the majority of component masses can be determined relative to the amount of cathode material present in the cell, the cathode mass was calculated first using an assumed, practical areal capacity of  $2 \text{ mAh cm}^{-2}$ .<sup>87</sup> Step-by-step example calculations are shown below for a NMC811-Graphite pouch cell. These steps can be adapted to any battery chemistry that contains the components previously listed.

## Pouch Cell Dimensions

**Table S1.** Areas of Pouch Cell Components<sup>88</sup>

Pouch Cell Component	Area (cm <sup>2</sup> )
Cathode	14.1
Anode	14.9
Separator <sup>a</sup>	14.9
Cell Casing	28.8

a: separator assumed to have the same area as the anode

## Step 1. List the Components

- **Positive Electrode**
  - NMC811
  - Carbon Black
  - PVDF Binder
  - Al foil current collector
  - NMP solvent
  
- **Negative Electrode**
  - Graphite
  - Carbon Black
  - CMC Binder
  - Cu foil current collector
  - Water solvent

- **Separator**
  - Polyethylene
  
- **Electrolyte**
  - Ethylene carbonate (EC)
  - Dimethyl carbonate (DMC)
  - LiPF<sub>6</sub> salt
  
- **Cell Casing**
  - Aluminum

### Step 2. Calculate Cathode Mass

Cathode Area: 14.1 cm<sup>2</sup>

NMC811 Gravimetric Capacity<sup>89</sup>: 180 mAh g<sup>-1</sup>

NMC811 Areal Capacity<sup>87</sup>: 2 mAh cm<sup>-2</sup>

$$\text{Mass of NMC811} = 14.1 \text{ cm}^2 * \frac{2 \text{ mAh}}{\text{cm}^2} * \frac{\text{g NMC811}}{180 \text{ mAh}} * 2 \text{ sides} = 0.313 \text{ g NMC811}$$

### Step 3. Calculate Remaining Positive Electrode Component Masses

Assumed Electrode Weight Distribution: 90% NMC811, 5% PVDF, 5% Carbon Black

Assumed NMP: PVDF mass ratio of 40.67 (gives a solids content of 45 wt.%)

Assumed 10 μm thick Al foil

$$\text{Mass of PVDF} = 0.313 \text{ g NMC811} * \frac{5 \text{ g PVDF}}{90 \text{ g NMC811}} = 0.0174 \text{ g PVDF}$$

$$\text{Mass of Carbon Black} = 0.313 \text{ g NMC811} * \frac{5 \text{ g Carbon Black}}{90 \text{ g NMC811}} = 0.0174 \text{ g Carbon Black}$$

$$\text{Mass of NMP} = 0.0174 \text{ g PVDF} * \frac{40.67 \text{ g NMP}}{\text{g PVDF}} = 0.707 \text{ g NMP}$$

$$\text{Mass of Al foil} = 14.1 \text{ cm}^2 * 10 \text{ μm} * \frac{10^{-4} \text{ cm}}{\text{μm}} * \frac{2.7 \text{ g Al}}{\text{cm}^3} = 0.0380 \text{ g Al}$$

### Step 4. Calculate Anode Mass

Assume N/P (negative/positive) ratio of 1.1

Graphite Gravimetric Capacity: 372 mAh g<sup>-1</sup>

Total Cathode Capacity: 56.34 mAh (calculated above for NMC811)

$$\text{Mass of Graphite} = 56.34 \text{ mAh} * 1.1 * \frac{\text{g Graphite}}{372 \text{ mAh}} = 0.167 \text{ g Graphite}$$

### Step 5. Calculate Remaining Negative Electrode Component Masses

Assumed Electrode Weight Distribution: 94% Graphite, 4% CMC, 2% Carbon Black

Assumed Water:CMC mass ratio of 40.67 (solids content of 45 wt.%)

Assumed 10 μm thick Cu foil

$$\text{Mass of CMC} = 0.167 \text{ g Graphite} * \frac{4 \text{ g CMC}}{94 \text{ g Graphite}} = 0.00709 \text{ g CMC}$$

$$\text{Mass of Carbon Black} = 0.167 \text{ g Graphite} * \frac{2 \text{ g Carbon Black}}{94 \text{ g Graphite}} = 0.00354 \text{ g Carbon Black}$$

$$\text{Mass of Water} = 0.00709 \text{ g CMC} * \frac{40.67 \text{ g Water}}{\text{g CMC}} = 0.288 \text{ g Water}$$

$$\text{Mass of Cu Foil} = 14.9 \text{ cm}^2 * 10 \text{ μm} * \frac{10^{-4} \text{ cm}}{\text{μm}} * \frac{8.96 \text{ g Cu}}{\text{cm}^3} * 2 \text{ Anodes} = 0.267 \text{ g Cu}$$

### Step 6. Calculate Separator Mass

Assumed 4 total layers of separator in pouch cell wrap (one between each pair of electrodes and one on each end of the electrode stack)

Assumed separator has the same area as the anode and 25.4 μm thickness<sup>90</sup>

$$\text{Mass of Separator} = 14.9 \text{ cm}^2 * 25.4 \text{ μm} * \frac{10^{-4} \text{ cm}}{\text{um}} * \frac{0.92 \text{ g PE}}{\text{cm}^3} * 4 \text{ layers} = 0.139 \text{ g PE}$$

### Step 7. Calculate Electrolyte Mass

Assumed 1 M LiPF<sub>6</sub> in 3:7 EC/DMC (wt. ratio)

Assumed electrolyte loading of 2.6 mL Ah<sup>-1</sup>.<sup>91</sup>

Assumed Electrolyte Density: 1.145 g mL<sup>-1</sup> (weighted average of EC and DMC)

$$\text{Total Electrolyte Mass} = 56.34 \text{ mAh} * \frac{\text{Ah}}{1000 \text{ mAh}} * \frac{2.6 \text{ mL}}{\text{Ah}} * \frac{1.145 \text{ g}}{\text{mL}} = 0.166 \text{ g Electrolyte}$$

$$\text{Mass of EC} = 0.166 \text{ g} * 0.3 = 0.0499 \text{ g EC}$$

$$\text{Mass of DMC} = 0.166 \text{ g} * 0.7 = 0.117 \text{ g DMC}$$

$$\text{Mass of LiPF}_6 = 0.166 \text{ g} * \frac{1 \text{ mL}}{1.145 \text{ g}} * \frac{\text{L}}{1000 \text{ mL}} * \frac{1 \text{ mol LiPF}_6}{\text{L}} * \frac{151.905 \text{ g}}{\text{mol}} = 0.0221 \text{ g LiPF}_6$$

### Step 8. Calculate Cell Casing Mass

Assumed cell casing is pure aluminum and 100 μm thick on each side

$$\text{Mass of Casing} = 28.8 \text{ cm}^2 * 100 \text{ } \mu\text{m} * \frac{10^{-4} \text{ cm}}{\mu\text{m}} * \frac{2.7 \text{ g Al}}{\text{cm}^3} * 2 \text{ sides} = 1.555 \text{ g Al}$$

**Table S2. Battery Component Mass Summary**

Component	Mass (g)
NMC811	0.313
Graphite	0.167
PVDF	0.0174
CMC	0.00709
Water	0.288
Carbon	0.0209
NMP	0.707
LiPF <sub>6</sub>	0.0221
EC	0.0499
DMC	0.117
Polyethylene	0.139
Aluminum	1.593
Copper	0.267

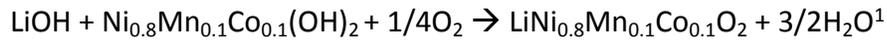
### **Heat Transfer and Heat Capacity Calculations**

Energy requirements for each intermediate reaction in the battery manufacturing process were assumed to be the sum of the heat needed to heat the reactants ( $Q_{\text{reactants}}$ ) and the heat needed to maintain the reactor temperature ( $Q_{\text{reactor}}$ ) (Equation S1).

$$Q_{\text{total}} = Q_{\text{reactants}} + Q_{\text{reactor}} \quad (\text{Equation S1})^1$$

### Calculating $Q_{\text{reactants}}$

Consider the following calcination reaction for the NMC811 cathode:



Reaction Temperature: 800 °C<sup>1</sup>

$Q_{\text{reactants}}$  is calculated as follows ( $\text{O}_2$  gas contribution was assumed to be negligible):

$$Q_{\text{reactants}} = n_{\text{LiOH}}C_{p,\text{LiOH}}(800\text{ °C} - 25\text{ °C}) + n_{\text{NMC(OH)}_2}C_{p,\text{NMC(OH)}_2}(800\text{ °C} - 25\text{ °C})$$

Heat capacities for many compounds are readily available through the NIST Chemistry Webbook. Link: <https://webbook.nist.gov/chemistry/>

Wherever available, the temperature dependence of heat capacity was accounted for using the Shomate Equation (coefficients are provided in the NIST Chemistry Webbook) (Equation S2). Overwhelmingly, however, the first coefficient (A) contributes the most to the heat capacity value regardless of temperature, so assuming a constant heat capacity would be a reasonable assumption.

$$\text{Shomate Equation: } C_p^\circ = A + B * t + C * t^2 + D * t^3 + E * \frac{1}{t^2}$$

Where t = temperature (T)/1000

Integrating the Shomate Equation for a reaction occurring at  $T_2$  with reactant heating from  $T_1$  (assumed to be room temp.) yields:

$$\frac{Q_{\text{reactants}}}{\text{mol}} = C_p \Delta T = A * (T_2 - T_1) + B * \left( \frac{t_2^2 - t_1^2}{2} \right) + C * \left( \frac{t_2^3 - t_1^3}{3} \right) + D * \left( \frac{t_2^4 - t_1^4}{4} \right) + E * \left( \frac{1}{t_1} - \frac{1}{t_2} \right)$$

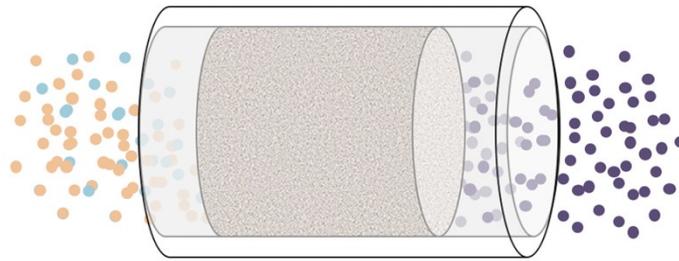
The Shomate Equation coefficients were used for  $C_{p,\text{LiOH}}$  and an assumed literature heat capacity for  $\text{Ni}(\text{OH})_2$  for  $C_{p,\text{NMC(OH)}_2}$  to determine  $Q_{\text{reactants}} = 0.313$  Btu for this reaction.

### Calculating $Q_{\text{reactor}}$

As mentioned in the article, it was assumed that the three possible reactors used in the battery manufacturing process are: (i) fixed bed reactor (gas-state reactions), (ii) batch reactor (liquid-state reactions), and (iii) tube furnace (solid-state reactions).

### Fixed Bed Reactor

In a fixed bed reactor, gas streams are passed into a cylinder that contains a packed catalyst bed. The gas molecules react in the presence of the catalyst to produce a product gas stream. These reactors are primarily used during the battery manufacturing process for production of petrochemicals from natural gas for synthesis of the separator and organic solvents.



**Fig. S1.** Fixed bed reactor.

The governing equation for  $Q_{\text{reactor}}$  of the fixed bed reactor is given below in Equation S2. This equation is an adaptation of Fourier's Law of Heat Conduction. It operates under the crucial assumption that the energy required to heat the reactor is equivalent to the energy removed from the reactor through conduction throughout the reaction. It was assumed that the reactors had no insulation, so this equation can be thought of as the upper bound energy requirement for a reaction.

$$Q_{\text{reactor, total rxn}} = \frac{kAt(T_{\text{rxn}} - 25^{\circ}\text{C})}{x} \quad \text{(Equation S2)}^1$$

$k$  = thermal conductivity  $\left(\frac{\text{W}}{\text{m} * \text{K}}\right)$ ;  $A$  = surface area ( $\text{m}^2$ );  $x$  = wall thickness (m);  $t$  = rxn time (s)

For simplicity, constant  $k$ ,  $A$ , and  $x$  values were assumed. As most gas phase reactions take place at high temperatures, the reactor was assumed to be made of stainless steel (rather than glass).

$$k = 16.26 \frac{\text{W}}{\text{m} * \text{K}} \text{ (stainless steel thermal conductivity)}^{92}$$

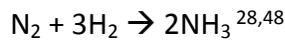
$A = 0.628 \text{ m}^2$  (for a 20 cm inner diameter, 100 cm long reactor)

$x = 0.00635 \text{ m}$  (0.25" thick; reasonable thickness for a reactor)

As fixed bed reactors are continuous reactors (reactants are continuously being sent into the reactor and products are continuously being produced), gas residence time (amount of time spent by a gas molecule in the reactor) is the most important metric for determining reaction energy requirement. Residence times for gas phase reactions involved in battery manufacturing were found in publications and patents.

The  $Q_{\text{reactor, total reaction}}$  value shown in Equation S2 is the total energy required to heat the reactor for a given amount of reactor operation time. Since fixed bed reactions are continuous as previously mentioned, the total energy requirement must be normalized to the amount of material reacted. This allows for determination of the amount of energy needed only to obtain the required amount of product for manufacturing the battery component, rather than the total amount of product produced. The total number of moles reacted can be calculated from the residence time value and reactor volume.

Consider the production of ammonia from  $N_2$  and  $H_2$  for NMP synthesis:



Reaction Temperature<sup>28,48</sup>: 425 °C

Residence Time (RT)<sup>28,48</sup>: 10 sec.

Volume of Reactor = 31415.9 cm<sup>3</sup> (based on dimensions previously given)

$$\text{Reactant Volumetric Flow Rate} = \frac{\text{Reactor Volume}}{RT} = \frac{31415.9 \text{ cm}^3}{10 \text{ s}} = 3141.59 \frac{\text{cm}^3}{\text{s}}$$

Density of  $N_2$  gas (assuming 25°C inlet) = 0.0012506 g cm<sup>-3</sup>

Density of  $H_2$  gas (assuming 25°C inlet) = 0.0000899 g cm<sup>-3</sup>

Molar weighted average reactant density = 0.00038 g cm<sup>-3</sup> (assumes inlet stream is 25 mol%  $N_2$  and 75 mol%  $H_2$ )

$$\text{Reactant Mass Flow Rate} = \frac{3141.59 \text{ cm}^3}{\text{s}} * \frac{0.00038 \text{ g}}{\text{cm}^3} = 1.194 \frac{\text{g}}{\text{s}}$$

Molar Mass of  $N_2$  = 28.014 g mol<sup>-1</sup>

Molar Mass of  $H_2$  = 2.016 g mol<sup>-1</sup>

$$\text{Reactant Molar Flow Rate} = 1.194 \frac{\text{g}}{\text{s}} * \left( 0.25 * \frac{\text{mol}}{28.014 \text{ g}} + 0.75 * \frac{\text{mol}}{2.016 \text{ g}} \right) = 0.455 \frac{\text{mol}}{\text{s}}$$

$$\text{Total Moles Reacted} = 0.455 \frac{\text{mol}}{\text{s}} * 3600 \text{ s} * 1 \text{ hr} = 1637.6 \text{ mol}$$

Assuming a total reaction time of 1 hour (this was assumed to be more than sufficient time to produce the necessary ammonia for manufacturing NMP for one battery pouch cell).

$$Q_{\text{reactor, total rxn}} = \frac{kAt(T_{\text{rxn}} - 25^\circ\text{C})}{x} = \frac{\left(16.26 \frac{\text{W}}{\text{m} * \text{K}}\right) * 0.628 \text{ m}^2 * 1 \text{ hr} * (425^\circ\text{C} - 25^\circ\text{C})}{0.00635 \text{ m}} = 2.32 * 10^9 \text{ J}$$

Normalizing  $Q_{\text{reactor, total rxn}}$  by the total moles reacted and multiplying by the number of moles of  $\text{N}_2/\text{H}_2$  gas reacted for the necessary ammonia production....

$$Q_{\text{reactor}} = \frac{2.32 * 10^9 \text{ J}}{1637.6 \text{ mol}} * 0.0143 \text{ mol} = 20,185 \text{ J} = 19.13 \text{ BTU}$$

### Batch Reactor

In a batch reactor, solid components are typically mixed in liquid media for a fixed amount of time during which a reaction proceeds. Unlike the fixed bed reactor, this reaction is not assumed to be continuous, so the calculations are somewhat simplified. The  $Q_{\text{reactor}}$  equation is identical to that of fixed bed reactor.



**Fig. S2.** Batch reactor.

$$Q_{\text{reactor, total rxn}} = \frac{kAt(T_{\text{rxn}} - 25^{\circ}\text{C})}{x}$$

Thermal conductivity  $\left(\frac{W}{m * K}\right)$ ; A = surface area ( $m^2$ ); x = wall thickness (m); t = rxn time (s)

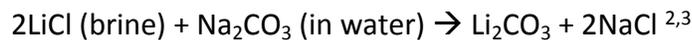
For simplicity, constant k, A, and x values were assumed. As liquid reactions can take place in either glass reactors or steel autoclaves, thermal conductivity values were given accordingly (the reactor types were straightforward to find in publications and patents).

$$k = 1.005 \left(\frac{W}{m * K}\right) \text{ for glass}^{92}; 16.26 \left(\frac{W}{m * K}\right) \text{ for stainless steel}^{92}$$

$$A = 0.0025 \text{ m}^2 \text{ (based on an assumed 1 L volume)}$$

$$x = 0.00635 \text{ m (0.25" thick)}$$

Consider the production of  $\text{Li}_2\text{CO}_3$  from LiCl brine



Reaction Temperature<sup>2,3</sup>:  $100^{\circ}\text{C}$

Reaction Time<sup>2,3</sup>: 2 hours

As with the fixed bed reactor, the energy required to heat the batch reactor must be normalized to the amount of reactant filled in the reactor.

Assuming 50% of the reactor can be filled with liquid, 0.5 L would be the liquid volume.

As this is taking place in water, it can be assumed that the liquid density is that of water ( $0.997 \text{ kg L}^{-1}$ ).

$$\text{Mass of Liquid} = 0.5 \text{ L} * \frac{0.997 \text{ kg}}{\text{L}} = 0.498 \text{ kg} = 498 \text{ g}$$

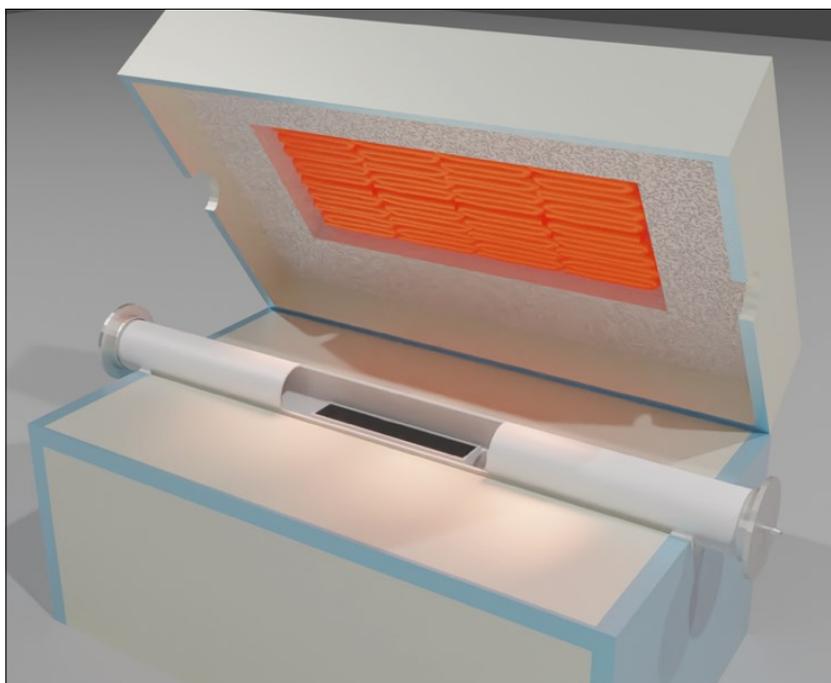
$$Q_{\text{reactor, total rxn}} = \frac{kAt(T_{\text{rxn}} - 25^{\circ}\text{C})}{x} = \frac{\left(1.005 \frac{W}{m * K}\right) * 0.0025 \text{ m}^2 * 2 \text{ hr} * (100^{\circ}\text{C} - 25^{\circ}\text{C})}{0.00635 \text{ m}} = 2.14 * 10^5 \text{ J}$$

Normalizing  $Q_{\text{reactor, total rxn}}$  by the total mass reacted and multiplying by the mass needed for one battery cell's lithium...

$$Q_{reactor} = \frac{2.14 * 10^5 J}{498 g} * 0.847 g = 363 J = 0.344 BTU$$

### Tube Furnace

Tube furnaces are used for solid-state reactions (such as the calcination of cathode materials) and heating solid powders to a certain temperature in either air or a specific atmosphere. For this article, rather than attempting to model a tube furnace from scratch, technical specifications from a furnace manufacturer were utilized to determine an energy requirement.



**Fig. S3.** Tube Furnace

Data from: <https://www.carbolite-gero.com/products/tube-furnace-range/universal-tube-furnaces/tf-range/>

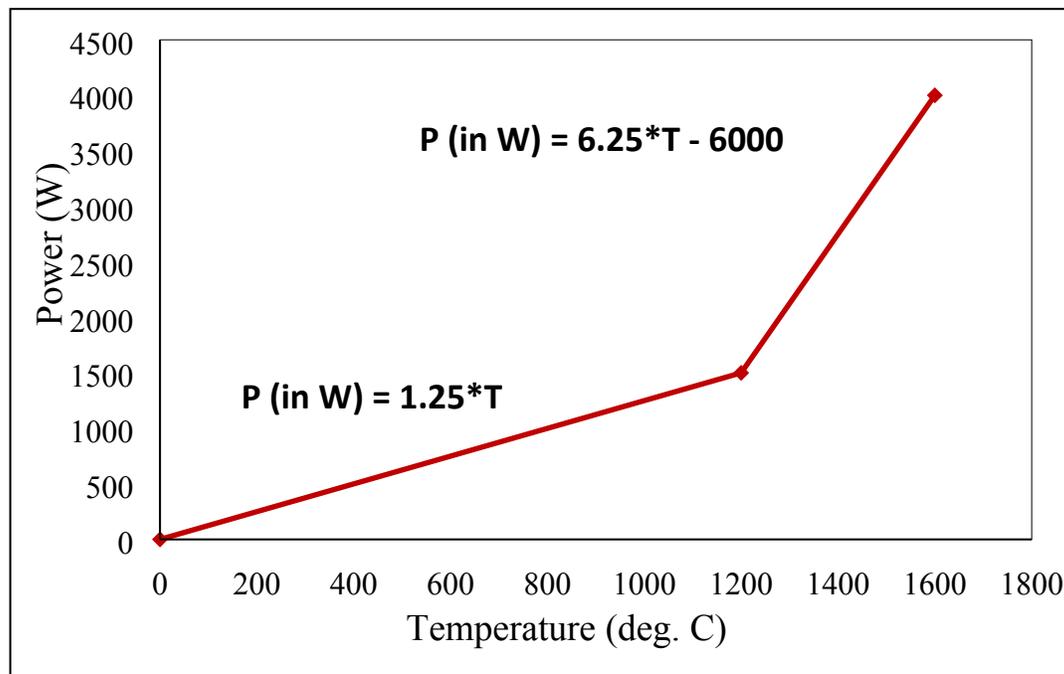
Maximum Temperature (°C)	Maximum Power (W)
0	0
1200	1500

$$P \text{ (in W)} = 1.25 * T \text{ (in } ^\circ\text{C)}$$

$$\text{for } 0 < T < 1200 \text{ } ^\circ\text{C}$$

Maximum Temperature (°C)	Maximum Power (W)
1200	1500

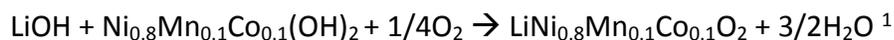
1600	4000
$P \text{ (in W)} = 6.25 * T - 6000 \text{ (in } ^\circ\text{C)}$	for $1200^\circ\text{C} < T$



**Fig. S4.** Furnace temperature vs. power approximation.

For a given reaction temperature, a power requirement was computed with the equations given above and assumed to be constant for the whole reaction.

Consider the calcination of  $\text{NMC}_{811}(\text{OH})_2$  and  $\text{LiOH}$  to yield  $\text{NMC}_{811}$



Reaction Conditions<sup>1</sup>: 450 °C for 12 hours, 800 °C for 8 hours

Furnace Heated Diameter: 60 mm

Furnace Heated Length: 300 mm

Heated Volume: 848.2 cm<sup>3</sup>

Assuming 50% of the heated volume can be filled with the solid reactants, the reactant volume would be 424.1 cm<sup>3</sup>.

LiOH density = 1.46 g cm<sup>-3</sup>

NMC811(OH)<sub>2</sub> density = 3.966 g cm<sup>-3</sup>

Weighted avg. density based on stoichiometry = 2.71 g cm<sup>-3</sup>

$$\text{Mass of Reactants} = 424.1 \text{ cm}^3 * \frac{2.71 \text{ g}}{\text{cm}^3} = 1150.5 \text{ g}$$

$$Q_{\text{reactor, total}} = \frac{562.5 \text{ J}}{\text{s}} * 3600 \text{ s} * 10 \text{ hr} + \frac{1000 \text{ J}}{\text{s}} * 3600 \text{ s} * 8 \text{ hr} = 4.91 * 10^7 \text{ J}$$

$$Q_{\text{reactor}} = \frac{4.91 * 10^7 \text{ J}}{1150.5 \text{ g}} * 0.372 \text{ g} = 15860 \text{ J} = 15 \text{ BTU}$$

## Raw Material Extraction Energy Calculations

### Open-Pit Mining

For materials obtained through open-pit mining, the energy use requirement was assumed to be entirely in the form of diesel fuel used to power mining equipment.<sup>93,94</sup> Based on the data from a GREET® technical report for cobalt mining life cycle analysis, a constant fuel requirement of ~ 425 gallons of diesel per kiloton of rock moved was assumed for all open-pit mining calculations.<sup>93,94</sup> As this fuel requirement is only with respect to the total amount of earth that needs to be extracted and moved during mining, the next step was to determine the fuel requirement with respect to the yield of the mineral of interest.

There are two factors that influence this fuel requirement calculation: stripping ratio and ore composition. Stripping ratio (SR) is defined as the ratio of the amount of waste rock removed to the amount of desired ore obtained. For example, in the case of cobalt mining, the Tenke Fungurume mine in the Democratic Republic of Congo has an estimated stripping ratio of 3.3, meaning 3.3 tons of waste rock must be removed to obtain one ton of cobalt-containing ore. In general, stripping ratios are widely available in the technical reports published by mining companies or through USGS Mineral Commodity Summaries. In addition to stripping ratio, ore composition also greatly influences the ultimate fuel requirement. For example, a cobalt-containing ore may have cobalt content of approximately 0.28% whereas a manganese-containing ore may have a manganese content of approximately 48%. Therefore, the yield of manganese per gallon of diesel fuel burned will be much greater than the yield of cobalt per gallon of diesel fuel burned. The effects of stripping ratio and ore composition are summarized in Equation S2, which was used in this article to determine mining fuel requirements.

$$\frac{\text{Gallons of diesel}}{\text{ton of mineral}} = \frac{0.425 \text{ gallons diesel}}{\text{ton}} * (1 + \text{SR}) * \frac{1}{\text{ore wt. frac.}} \quad (\text{Equation S2})$$

### Consider a nickel sulfide mining operation

Stripping ratio<sup>95</sup>: 1.3

Ore wt. fraction<sup>95</sup>: 0.0015 (1.5%)

Mass of nickel sulfide needed for NMC811: 0.232 g

$$\begin{aligned} \text{Diesel used} &= \frac{0.425 \text{ gal diesel}}{\text{ton}} * (1 + 1.3) * \frac{1}{0.0015} * \frac{1 \text{ ton}}{2000 \text{ lb}} * \frac{1 \text{ lb}}{453.59 \text{ g}} * 0.232 \text{ g} = 1.67 \end{aligned}$$

$$\text{Extraction Energy} = 1.67 * 10^{-4} \text{ gallons} * \frac{137380 \text{ Btu}}{\text{gallon}} = 22.9 \text{ BTU}$$

### Oil & Natural Gas Extraction

In order to compute the energy requirements for oil & gas extraction, a quantity known as the “energy return on investment” (EROI) was utilized. EROI is defined as the ratio of the energy extracted to the energy put in. For example, an EROI of 10 means that 10 units of energy can be extracted per unit of energy used. Therefore, the higher the EROI, the less the required energy input. For this article, natural gas and petroleum were assumed to have EROIs of 43.5 and 20, respectively.<sup>96</sup> It should be noted that these values can vary significantly between extraction sites.

### Consider a natural gas extraction operation (for production of the PE separator)

EROI<sup>96</sup>: 43.5

Ethane content in natural gas<sup>97</sup>: 4.2%

Mass of ethane required: 0.149 g

$$\text{Mass of Fuel Needed} = 0.149 \text{ g ethane} * \frac{1 \text{ g NG}}{0.042 \text{ g ethane}} * \frac{1 \text{ g fuel}}{43.5 \text{ g NG}} = 0.081 \text{ g fuel}$$

$$\text{Extraction Energy} = 0.081 \text{ g} * \frac{1 \text{ gal diesel}}{3220.489 \text{ g}} * \frac{137380 \text{ BTU}}{\text{gallon}} = 3.49 \text{ BTU}$$

## Brine Evaporation

As this technique relies on solar evaporation of brine pools, it is assumed to have a negligible energy input requirement.

## **Transportation Energy Calculations**

Materials transportation also requires significant energy. For example, for a Li-ion battery, cobalt is typically obtained from the DRC, graphite from China, and lithium from Chile/Argentina (Figure 2). Therefore, cargo ships and freight trains are needed to transport these materials from their sources to where they are processed and used for syntheses (assumed to be Austin, TX in this article). A map distance calculator between cities was used to approximate the distance a cargo ship/freight train would have to travel from the raw material source to Austin, TX. For compounds that are readily available in the United States and aren't imported in significant volume (*i.e.*, sodium, natural gas, coal, *etc.*), transportation energy requirements were assumed to be negligible. Literature values for the energy required to transport raw materials by cargo ship ( $411 \text{ Btu ton}^{-1} \text{ mile}^{-1}$ ) or freight train ( $371 \text{ Btu ton}^{-1} \text{ mile}^{-1}$ ) were used in the calculations.<sup>98</sup> These values were multiplied by the distance traveled and the mass of the material being transported to obtain an energy requirement.

Sea Distance Calculator (cargo ship): <https://sea-distances.org/>

Land Distance Calculator (freight train): any map software

Consider cobalt being transported from the DRC to Texas

Primary mode of transport: cargo ship

Distance (as determined by sea distance calculator): 7552 miles

One major challenge with determining transportation energy requirements is that there is no way to generally know how much of the mineral of the interest is on a given cargo ship. For example, a cargo ship could contain entirely cobalt, meaning the fuel burned is exclusively for cobalt transport. On the other hand, a cargo ship may only contain one container of cobalt, meaning very little cobalt is actually transported for the amount of fuel burned. For this article, a "raw material of interest" content of 42.5% was assumed for all cargo ship/freight train calculations as this is the estimated share that "dry bulk cargo" makes up of total global shipping.<sup>99</sup>

$$\text{Transport Energy} = \frac{411 \text{ Btu}}{\text{ton} * \text{mile}} * \frac{1 \text{ ton}}{2000 \text{ lb}} * \frac{1 \text{ lb}}{453.59 \text{ g}} * \frac{1}{0.425} * 0.029 \text{ g CoS} * 7552 \text{ mi} = 0.234 \text{ BTU}$$

## Translating Energy to Emissions with GREET®

After obtaining the energy requirements for manufacturing, extraction, and transportation, the data included in the GREET® model (GREET2 spreadsheet) was used to convert energy to emissions. The emissions quantities obtained included: CO<sub>2</sub>, CH<sub>4</sub>, SO<sub>x</sub>, NO<sub>x</sub>, PM<sub>2.5</sub>, PM<sub>10</sub> and more. The electricity fuel mix was also varied to compare emissions with the current fuel mix to future fuel mixes where clean energy technologies make up a larger share. Transportation and raw material extraction emissions were obtained using the GREET® values for bunker fuel and diesel fuel.<sup>[13]</sup> Data, such as that included for natural gas below, were used to simply transform BTU of energy used into grams of emissions. For simplicity, all manufacturing reaction energy was assumed to be in the form of electricity (a mix of NG, coal, clean, etc.) Data for all fuel types were included in the GREET2 spreadsheet. A weighted average of the fuel types was used to determine to total emissions for a given fuel mix.

GREET2 Spreadsheet: <https://greet.es.anl.gov/>

**Table S3.** Emissions Values for a natural gas boiler from GREET2 spreadsheet

Natural Gas	
Emission Category	Utility/Industrial Boiler (g/mmBTU)
VOC	2.54
CO	22.21
NO <sub>x</sub>	36.4
PM10	3.507
PM2.5	3.507
SO <sub>x</sub>	0.269
BC	0.579
OC	1.501
CH <sub>4</sub>	1.06
N <sub>2</sub> O	0.75
CO <sub>2</sub>	59367

## Toxicity Scoring

The Globally Harmonized System (GHS) of Classification and Labeling of Chemicals was used to assess battery toxicity. The following seven toxicity topics are considered in the analysis: acute

oral toxicity, acute dermal toxicity, acute inhalation toxicity, carcinogenicity, acute aquatic toxicity, chronic aquatic toxicity, and ozone layer depletion. For a given chemical, if there is considered a risk for any of those topics, the chemical is assigned a GHS category classification. Lower category numbers correspond to higher risk (typically increased by an order of magnitude between categories). Only categories 1, 2, and 3 were considered in the scope of this article as lower categories than that are considered lower risk. Scores were assigned as follows:

#### **Acute oral toxicity, Acute dermal toxicity, and Acute inhalation toxicity**

Category 1: 0.1

Category 2: 0.01

Category 3: 0.001

#### **Acute aquatic toxicity and Chronic aquatic toxicity**

Category 1: 0.1

Category 2: 0.01

Category 3: 0.001

#### **Carcinogenicity**

Category 1: 0.1

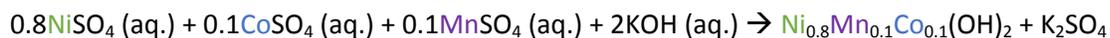
Category 2: 0.01

#### **Ozone Layer Depletion**

Category 1: 0.1

Maximum possible score for a compound: **0.7**

Consider the following NMC co-precipitation reaction



The chemicals present are as follows: NiSO<sub>4</sub>, CoSO<sub>4</sub>, MnSO<sub>4</sub>, KOH, NMC(OH)<sub>2</sub>, K<sub>2</sub>SO<sub>4</sub>. GHS labeling for **EVERY** compound present in the reaction was obtained. The PubChem Database is comprehensive, open-access resource for GHS labeling. Link: <https://pubchem.ncbi.nlm.nih.gov/>

Pictogram(s)	   Irritant      Health Hazard      Environmental Hazard
Signal	<b>Danger</b>
GHS Hazard Statements	H302: Harmful if swallowed [ <b>Warning</b> Acute toxicity, oral] H315: Causes skin irritation [ <b>Warning</b> Skin corrosion/irritation] H317: May cause an allergic skin reaction [ <b>Warning</b> Sensitization, Skin] H332: Harmful if inhaled [ <b>Warning</b> Acute toxicity, inhalation] H334: May cause allergy or asthma symptoms or breathing difficulties if inhaled [ <b>Danger</b> Sensitization, respiratory] H341: Suspected of causing genetic defects [ <b>Warning</b> Germ cell mutagenicity] H350i: May cause cancer by inhalation [ <b>Danger</b> Carcinogenicity] H360D ***: May damage the unborn child [ <b>Danger</b> Reproductive toxicity] H372 **: Causes damage to organs through prolonged or repeated exposure [ <b>Danger</b> Specific target organ toxicity, repeated exposure] H400: Very toxic to aquatic life [ <b>Warning</b> Hazardous to the aquatic environment, acute hazard] H410: Very toxic to aquatic life with long lasting effects [ <b>Warning</b> Hazardous to the aquatic environment, long-term hazard]

**Fig. S5.** Example GHS chemical label for NiSO<sub>4</sub>.

Figure S5 above shows an example GHS statement for NiSO<sub>4</sub> obtained from the PubChem database. As shown in the label, hazard statements are present for the following categories: acute oral toxicity, acute inhalation toxicity, carcinogenicity, acute aquatic toxicity, and chronic aquatic toxicity (5 of the 7 topics).

The GHS hazard statement code can be paired with a category number through the GHS classification found here: <https://pubchem.ncbi.nlm.nih.gov/ghs/>

H400	Very toxic to aquatic life	Hazardous to the aquatic environment, acute hazard	Category 1		<b>Warning</b>	P273	P391	P501
H401	Toxic to aquatic life	Hazardous to the aquatic environment, acute hazard	Category 2	None		P273		P501
H402	Harmful to aquatic life	Hazardous to the aquatic environment, acute hazard	Category 3	None		P273		P501
H410	Very toxic to aquatic life with long lasting effects	Hazardous to the aquatic environment, long-term hazard	Category 1		<b>Warning</b>	P273	P391	P501
H411	Toxic to aquatic life with long lasting effects	Hazardous to the aquatic environment, long-term hazard	Category 2			P273	P391	P501
H412	Harmful to aquatic life with long lasting effects	Hazardous to the aquatic environment, long-term hazard	Category 3	None		P273		P501

**Fig. S6.** GHS category classification from codes for aquatic toxicity topic.

Category classification corresponding to the GHS hazard statement codes is shown for the aquatic toxicity topic in Figure S6. For NiSO<sub>4</sub>, codes H400 and H410 are present in the chemical label, corresponding to category 1 toxicity for both acute and chronic aquatic toxicity. Therefore, a score of 0.1 will be given to NiSO<sub>4</sub> for each of these categories. This process is repeated for all hazard statements that are present to get a total toxicity score for the compound. This process is continued for all compounds present in the battery manufacturing process.

## Habitat Destruction Quantification

The third category included in this article's framework is habitat destruction. For these calculations, technical reports regarding mining, oil & gas extraction, and brine extraction operations were used to estimate raw material yield per area of land used (*i.e.*, tons km<sup>-2</sup>). For example, in the case of cobalt mining, a technical report from Katanga Mining Limited, one of the primary cobalt mining companies in the DRC, was obtained. For one of Katanga Mining Limited's operational mining areas, the report stated that 8.49 km<sup>2</sup> of land was being utilized for cobalt mining and the site contained an estimated 227,840 tons of cobalt reserves. Therefore, it was assumed that the cobalt yield was ~ 26,800 tons km<sup>-2</sup>.<sup>100</sup> For each raw material used in the battery, a yield per area value was obtained from technical reports and the amount of each material needed was divided by this value to determine a habitat destruction value. It is worth acknowledging that raw material yield can vary significantly from site to site. Therefore, wherever possible, technical reports from prominent extraction sites were used (*i.e.*, cobalt mines in the DRC, lithium brine in Argentina, *etc.*).<sup>101</sup>

Consider the cobalt in an NMC811 cathode

$$\text{CoS Mining Land Use} = \frac{1 \text{ km}^2}{26,800 \text{ tons CoS}} * \frac{1 \text{ ton}}{2000 \text{ lb}} * \frac{1 \text{ lb}}{453.59 \text{ g}} * 0.029 \text{ g CoS} = 1.2 * 10^{-6} \text{ m}^2$$

This procedure was repeated for all "raw materials" involved in the production of a battery (*i.e.*, transition metals, oil & gas, brine, *etc.*)

## Social Impact Assessment

Social impact is notoriously difficult to evaluate quantitatively. A straightforward social impact assessment methodology commonly used in the literature is the simple listing and discussion of potential negative social impacts. Therefore, for the purpose of this article, this category involves entirely qualitative analyses of newspaper articles, investigative reports, commentary from human rights organizations, and interviews from community members. The Business & Human Rights Resource Centre's (a registered 501(c)(3) non-profit organization) database was used to search for and access an accumulated list of articles, reports, *etc.* For example, the phrase "cobalt mining" was queried in the database and dozens of resources related to human rights violations in the DRC were obtained.<sup>40</sup> The resources that appeared to be from the most reputable sources were then reviewed, and a list of some of the detrimental social impacts of cobalt mining was compiled. This process was repeated for all key raw materials used in the manufacturing of the battery components.

Business & Human Rights Resource Centre Link: <https://www.business-humanrights.org/>

# NMC811-Graphite Manufacturing Process

## LiNi<sub>0.8</sub>Mn<sub>0.1</sub>Co<sub>0.1</sub>O<sub>2</sub> – Graphite Pouch Cell

Only tracing each element (or functional group) in the final compound.

$$Q = A(T_2 - T_1) + B(T_2^2 - T_1^2)/2 + C(T_2^3 - T_1^3)/3 + D(T_2^4 - T_1^4)/4 - E((1/T_2) - (1/T_1))$$

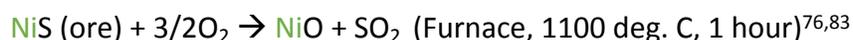
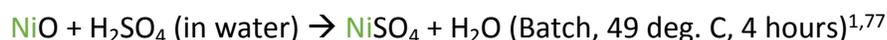
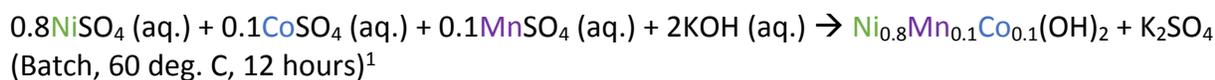
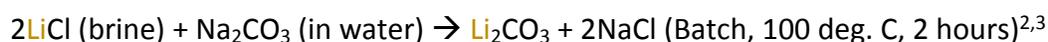
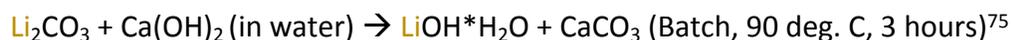
$$Q_{\text{total}} = Q_{\text{vessel}} + Q_{\text{precursors}}$$

Types of reactors: Furnace (solid), Batch (liquid), Fixed Bed (gas)

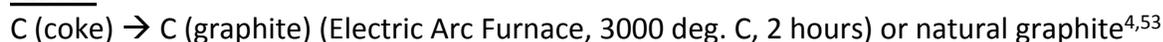
(Vessel Type, Reaction Temperature, Time Held at Temperature)

For unknown residence times, 0.1 sec. was assumed.

### Cathode



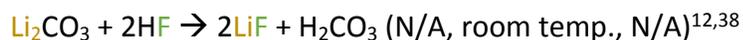
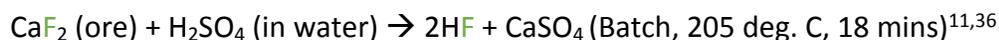
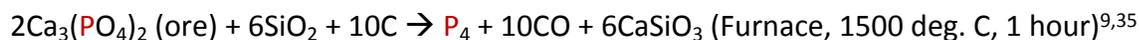
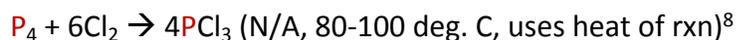
### Anode



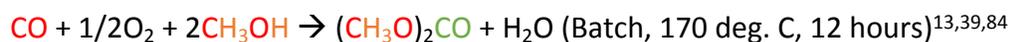
## Electrolyte

$\text{LiPF}_6$  in  $(\text{CH}_3\text{O})_2\text{CO}$  and  $(\text{CH}_2\text{O})_2\text{CO}$

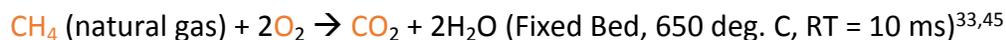
$\text{LiPF}_6$



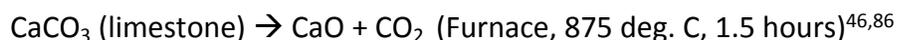
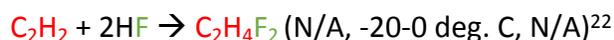
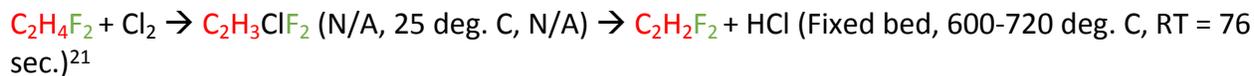
$(\text{CH}_3\text{O})_2\text{CO}$  (DMC)



$(\text{CH}_2\text{O})_2\text{CO}$  (EC)



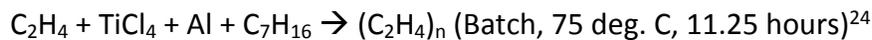
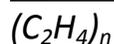
## **Binder**



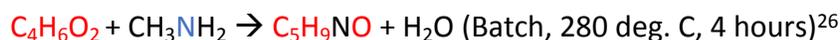
## **CMC**



## **Separator**



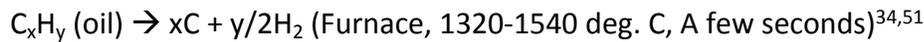
## **Solvent**





### Conductive additives

#### *Carbon Black*



### Other components (from GREET)

Current collectors: Al, Cu

Casing: Al

## **LFP-Graphite Manufacturing Process**

### **LiFePO<sub>4</sub> – Graphite Pouch Cell**

Only tracing each element (or functional group) in the final compound.

$$Q = A(T_2 - T_1) + B(T_2^2 - T_1^2)/2 + C(T_2^3 - T_1^3)/3 + D(T_2^4 - T_1^4)/4 - E((1/T_2) - (1/T_1))$$

$$Q_{\text{total}} = Q_{\text{vessel}} + Q_{\text{precursors}}$$

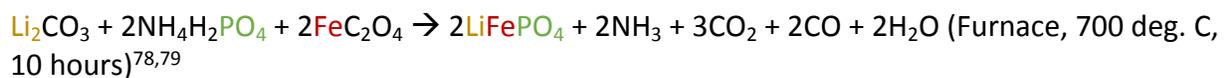
Types of reactors: Furnace (solid), Batch (liquid), Fixed Bed (gas)

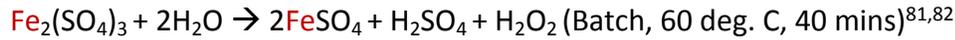
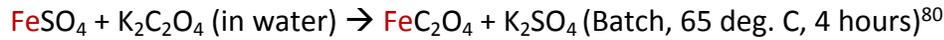
(Vessel Type, Reaction Temperature, Time Held at Temperature)

For unknown residence times, 0.1 sec. was assumed.

### Cathode

#### **LiFePO<sub>4</sub>**





\*\*\* All other components are the same as NMC811-Graphite

## Aqueous Na-ion Manufacturing Process

### Na<sub>0.44</sub>MnO<sub>2</sub> - NaTi<sub>2</sub>(PO<sub>4</sub>)<sub>3</sub> Pouch Cell

Only tracing each element (or function group) in the final compound.

$$Q = A(T_2 - T_1) + B(T_2^2 - T_1^2)/2 + C(T_2^3 - T_1^3)/3 + D(T_2^4 - T_1^4)/4 - E((1/T_2) - (1/T_1))$$

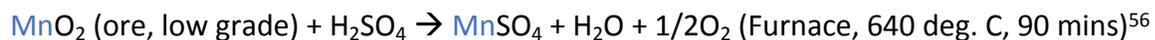
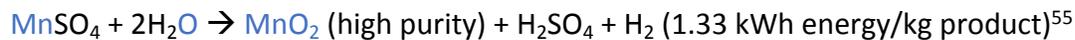
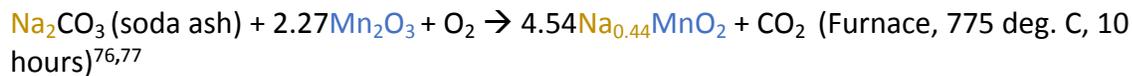
$$Q_{\text{total}} = Q_{\text{vessel}} + Q_{\text{precursors}}$$

Types of reactors: Furnace (solid), CSTR (liquid), Fixed Bed (gas)

(Vessel Type, Reaction Temperature, Time Held at Temperature)

For unknown residence times, 0.1 sec. was assumed.

#### Cathode



#### Anode



$\text{NaH}_2\text{PO}_4 + 2\text{TiO}_2 + 2(\text{NH}_4)_2\text{HPO}_4 \rightarrow \text{NaTi}_2(\text{PO}_4)_3 + 4\text{NH}_3 + 4\text{H}_2\text{O}$  (Furnace, 300 deg. C for 1 hr + 950 deg. C for 2 hrs)<sup>57</sup>

$\text{NaCl}$  (seawater/brine) +  $\text{H}_3\text{PO}_4$  (in water)  $\rightarrow \text{NaH}_2\text{PO}_4 + \text{HCl}$  (CSTR, 115 deg. C, 24 hrs)<sup>58</sup>

$\text{Ca}_5(\text{PO}_4)_3\text{OH}$  (ore) +  $5\text{H}_2\text{SO}_4$  (in water)  $\rightarrow 3\text{H}_3\text{PO}_4 + 5\text{CaSO}_4 + \text{H}_2\text{O}$  (CSTR, 85 deg. C, 1 hour)<sup>59</sup>

$\text{FeTiO}_3$  (ore) +  $2\text{H}_2\text{SO}_4$  (in water)  $\rightarrow \text{TiOSO}_4 + \text{FeSO}_4 + 2\text{H}_2\text{O}$  (CSTR, 150 deg. C, 2.5 hr)<sup>60,62,63</sup>

$\text{TiOSO}_4 + \text{H}_2\text{O} \rightarrow \text{TiO}_2 \cdot n\text{H}_2\text{O} + \text{H}_2\text{SO}_4$  (CSTR, 110 deg. C, 1 hr)<sup>60,62</sup>

$\text{TiO}_2 \cdot n\text{H}_2\text{O} \rightarrow \text{TiO}_2 + \text{H}_2\text{O}$  (Furnace, 830 deg. C, 2.5 hrs)<sup>60,61</sup>

$\text{NH}_3 + \text{H}_3\text{PO}_4 \rightarrow \text{NH}_4\text{H}_2\text{PO}_4$  (PFR, 305 deg. C, RT = 0.14 sec)<sup>64</sup>

$\text{Ca}_5(\text{PO}_4)_3\text{OH}$  (ore) +  $5\text{H}_2\text{SO}_4$  (in water)  $\rightarrow 3\text{H}_3\text{PO}_4 + 5\text{CaSO}_4 + \text{H}_2\text{O}$  (CSTR, 85 deg. C, 1 hour)<sup>59</sup>

$\text{NH}_4\text{H}_2\text{PO}_4 + \text{NH}_3$  (in water)  $\rightarrow (\text{NH}_4)_2\text{HPO}_4$  (CSTR, 86 deg. C, 30 mins)<sup>65</sup>

### **Binder**

$(\text{C}_2\text{F}_4)_n$

$\text{C}_2\text{F}_4 + (\text{NH}_4)_2\text{S}_2\text{O}_8$  (0.1% mass of TFE) +  $\text{Na}_2\text{B}_4\text{O}_7 \cdot 10\text{H}_2\text{O}$  (0.75% mass of TFE) +  $\text{H}_2\text{O} \rightarrow (\text{C}_2\text{F}_4)_n$  (CSTR (autoclave), 70 deg. C, 176 min.)<sup>66,67</sup>

$\text{CHCl}_3 + 2\text{HF} \rightarrow \text{CHClF}_2 + 2\text{HCl}$  (CSTR, 80 deg. C, 2 hours)<sup>66,68</sup>

$2\text{CHClF}_2 \rightarrow \text{C}_2\text{F}_4 + 2\text{HCl}$  (PFR, 750-950 deg. C, RT = 0.05 s)<sup>66,69</sup>

$\text{CaF}_2$  (ore) +  $\text{H}_2\text{SO}_4 \rightarrow 2\text{HF} + \text{CaSO}_4$  (CSTR, 205 deg. C, 20 mins)<sup>11,36</sup>

$\text{CCl}_4 + \text{H}_2 \rightarrow \text{CHCl}_3 + \text{HCl}$  (PFR, 80 deg. C, RT = 5 s)<sup>70</sup>

$\text{CH}_4$  (natural gas) +  $\text{Cl}_2 \rightarrow \text{CCl}_4 + 4\text{HCl}$  (N/A, 25 deg. C, N/A)<sup>71</sup>

### **Graphite**

C (coke)  $\rightarrow$  C (graphite) (Electric Arc Furnace, 3000 deg. C, 2 hours) or natural graphite<sup>4,53</sup>

### **Carbon Black**

$\text{C}_x\text{H}_y$  (oil)  $\rightarrow x\text{C}$  (carbon black) +  $y/2\text{H}_2$  (Furnace, 1320-1540 deg. C, A few seconds)<sup>34,51</sup>

### **Activated Carbon**

$C_6H_{12}O_6$  (glucose)  $\rightarrow$  6C (activated carbon) + 6H<sub>2</sub>O (Furnace, 600 deg. C for 2 hrs + 800 deg. C for 2 hrs)<sup>54</sup>

### **Cotton**

Cotton is grown and spun into textiles. No thermal energy requirement is noted for this process.

### **Electrolyte**

1 M Na<sub>2</sub>SO<sub>4</sub> in H<sub>2</sub>O

Na<sub>2</sub>SO<sub>4</sub>\*10H<sub>2</sub>O (rock)  $\rightarrow$  Na<sub>2</sub>SO<sub>4</sub> + 10H<sub>2</sub>O (Furnace, 85 deg. C, 0.5 hrs bc quick process)<sup>72</sup>

H<sub>2</sub>O (brackish)  $\rightarrow$  H<sub>2</sub>O (deionized) (~2 kWh/m<sup>3</sup> of water produced)<sup>73</sup>

### **Pressing Energy**

In lieu of solvent, it is the energy required to stamp into free-standing electrodes. Using GREET data for stamping steel for now (stamping powder almost certainly takes less energy so this can be the max. upper bound). Stamping energy: 0.860 mmBtu/ton.<sup>74</sup>

### **Stainless Steel (Current Collector)**

From GREET2: 24.573 mmBtu/ton of material + 3.461 mmBtu/ton of material (cold rolling)

### **Polypropylene Casing**

From GREET2: 9.318 mmBtu/ton of material + 2.168 mmBtu/ton of material (extrusion)

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