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# Method for Predicting the Energy Characteristics of Li-Ion Cells Designed for High Specific Energy

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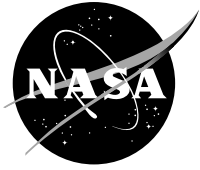
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# Method for Predicting the Energy Characteristics of Li-Ion Cells Designed for High Specific Energy

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## Abstract

Novel electrode materials with increased specific capacity and voltage performance are critical to the NASA goals for developing Li-ion batteries with increased specific energy and energy density. Although performance metrics of the individual electrodes are critically important, a fundamental understanding of the interactions of electrodes in a full cell is essential to achieving the desired performance, and for establishing meaningful goals for electrode performance in the first place. This paper presents design considerations for matching positive and negative electrodes in a viable design. Methods for predicting cell-level performance, based on laboratory data for individual electrodes, are presented and discussed.

## 1.0 Introduction

NASA's High Efficiency Space Power Systems (HESPS) Project is developing advanced lithium-ion cells for future NASA exploration missions under the Enabling Technology Development and Demonstration (ETDD) Program. This work, which began under the Exploration Technology Development Program (ETDP) Energy Storage Project, combines the efforts of industrial partners and contractors to develop aerospace cell designs with enhanced specific energy and safety characteristics (Ref. 1).

A spreadsheet model was developed to predict cell-level specific energy under relevant operating conditions, and to perform "what-if?" analysis for different cell materials and designs. Estimates of the cell discharge voltage profile use laboratory data for anodes and cathodes under relevant rates and temperatures. Cells are being developed to have a 35 Ah capacity when discharged at a C/10 rate to 3 V at 0 °C—in alignment with the stated ETDP key performance parameters (KPPs). Laboratory data for the individual electrodes in half-cells, collected at 0 °C and C/10 rates, are used to project capacity and energy at reduced temperature.

Key assumptions:

- Prismatic cells sized to deliver 35 Ah capacity with discharge to 3 V at 0°C
- Energy/capacity estimated for C/10 discharge rates
- Use electrode specific capacity observed in laboratory testing with limited number of cycles (neglects capacity loss with cycling)

- Scale electrode area to produce practical loading of active material on the foil current collector substrate
- Positive electrode porosity = 30 percent
- Negative electrode porosity = 35 percent
- Neglect electrode expansion with state of charge

Electrode loading—the quantity of active material per unit area of electrode—has a significant impact on cell performance and specific energy. Low loading levels require large electrode area and a greater mass of current collector foil. This situation is favorable for cells designed for high power applications, but produces a heavy cell with relatively low specific energy. High loading levels reduce current collector mass, but if the electrode layer becomes too thick, the utilization of electrode material at practical rates can be compromised. Optimization of loading level requires experimentation, but practical loadings are generally around 3 mAh/cm<sup>2</sup>. Moshtev and Johnson (Ref. 2) presented a physical analysis of commercial lithium-ion cells (c. 1999) which shows electrode-loading levels ranging from 2.4 to 3.4 mAh/cm<sup>2</sup>.

Physical cell design assumes a 0.5 mm thick aluminum case with 73 electrode pairs. The electrodes consist of alternating positive and negative electrode plates. The electrode plates are coated on both sides. The choice of the number of electrode pairs influences the number of internal tab connections as well as the thickness of the finished cell. The weight of case material is minimized when the cell shape is a cube. However, this geometry produces a thick cell with a large number of internal tab connections, and adds complexity to the assembly process. The choice of 73 pairs was believed to be representative of practical commercial prismatic cells. Cell construction is illustrated in Figure 1. Electrode tabs are joined together in the header space between the electrode top edge and the inside of the cover. Height, width and thickness are defined in Figure 1.

The electrode aspect ratio is assumed to be 1.5 (H/W). This choice produces a tall cell with reduced width and helps to reduce the volume of the header space at the "top" of the cell. Note that the cell in Figure 1 has an electrode aspect ratio that is less than one. Heat transfer and current distribution are also affected by the choice of aspect ratio. This effort neglected these effects.

Mass calculations include allowance for terminals, feed-through seals and internal tab connections. These are based on inspection of practical commercial cells of similar capacity. The cell mass includes allowance for 30 percent excess

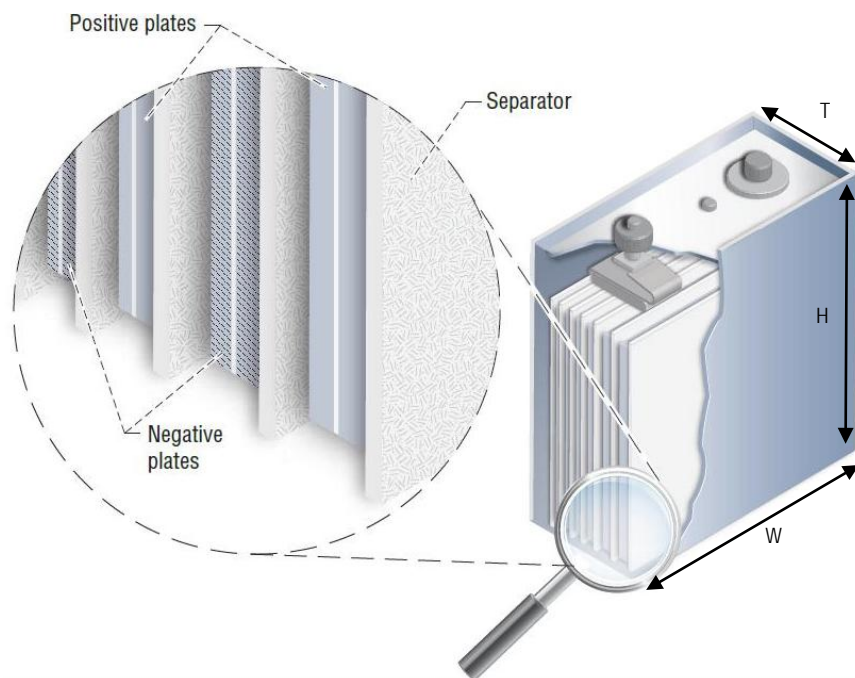


Figure 1.—Prismatic cell construction.

electrolyte, relative to the amount required to exactly fill the porous volume of the electrodes and separator material. This measure assures that the electrodes and separators are fully imbedded with electrolyte during the life of the cell. Negative electrodes and separators are assumed to be 2 mm larger than the positive electrode (all around) to prevent edge contact and short-circuiting inside the cell. The spreadsheet model assumes that the separator film covers the entire face of the oversized, negative electrodes. Alternatively, the smaller positive electrode may be enclosed in a separator pouch, resulting in less separator material.

Calculations use the density of the electrode components and the assumed porosity of the electrode layers to compute the total volume of electrode material. The assumed electrode area, aspect ratio and number of plates establish the dimensions of the electrode package. The cell model computes the mass of the case material required to enclose the cell bundle, with user-specified clearance at the edges, base and header space of the cell. The mass of internal tab connections is computed to reflect the number of electrode pairs.

Testing of the individual electrodes provides capacity and discharge voltage data that is used to forecast cell-level combinations. This report discusses the details of the forecasting methods that are used. Sample calculations are presented for state-of-the-art graphite and layered cathode material.

## 2.0 Performance of Single Electrodes in Half-Cells

### 2.1 Testing Considerations

Testing of the single electrodes is performed in half-cells with lithium metal counter-electrodes. Voltage limits for formation and cycling are based on anticipated maximum useable potential windows for the electrode materials under study. These potential windows represent the full utilization (maximum specific capacity) of the electrode material. Capacity matching, and the choice of P/N ratio, limits the useable electrode potential window in full cells. This will be illustrated in the example, which follows.

### 2.2 Typical Electrode Data

Screening of lithium-ion electrodes is usually performed in half-cells with lithium metal counter-electrodes having a substantial excess capacity relative to the electrode under study. The lithium counter-electrode serves as a pseudo-reference electrode, providing data for the individual electrode voltage versus lithium. Laboratory data for the first three cycles of practical, state-of-the-art positive and negative electrodes appears in Figure 2.

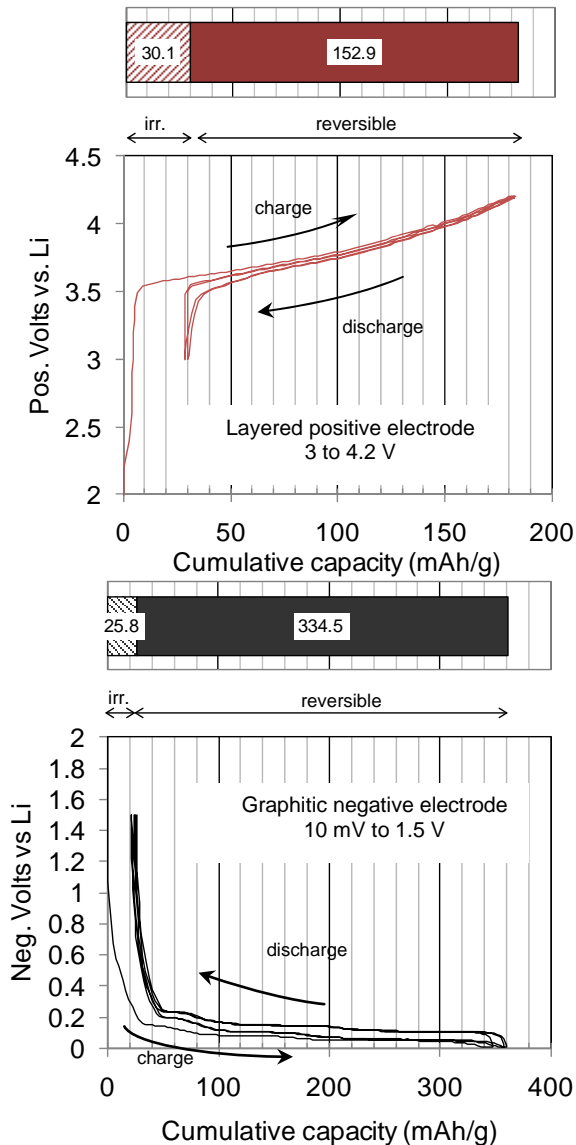


Figure 2.—The first three charge/discharge cycles of a positive and negative electrode in half-cells with lithium metal. Electrode potential versus specific capacity in mAh per gram of active material. Data at room temperature.

Figure 2 presents electrode potential as a function of the cumulative capacity (a running total of the charge capacity minus the discharge capacity over several cycles). On charge, the positive electrode is delithiated and becomes more positive. At the same time, the negative electrode accepts lithium ions on charge and becomes more negative. On discharge, the process is reversed. For both electrodes, the total first charge capacity is noticeably greater than the discharge capacity. The difference between cumulative charge and discharge capacity is defined as the irreversible capacity of the electrode. The reversible capacity is the capacity that is available to the load after the electrode

is formed. The total capacity absorbed by the electrode is the sum of the reversible and irreversible capacity.

For the positive electrode in Figure 2, a cumulative total capacity of 183 mAh/g is absorbed in the first few cycles. The reversible capacity is 153 mAh/g. The irreversible capacity of 30.1 mAh/g is equivalent to 19.7 percent of the reversible capacity.

Similarly, the negative electrode absorbs a cumulative charge capacity of 334 mAh/g. The irreversible capacity of 26 mAh/g is equivalent to 7.7 percent of the reversible capacity. The specific capacity for the Figure 2 electrodes is summarized in Table 1.

TABLE 1.—SPECIFIC CAPACITIES OF ELECTRODES IN mAh/g

	Positive	Negative
Irreversible	30.1	25.8
Reversible	152.9	334.5
Total	183.0	360.3
Irreversible (% of rev)	19.7%	7.7%

The reversible specific capacity is used to compute the electrode active material mass that is necessary to meet a desired electrode capacity. When performing cell-level calculations for capacity-balanced electrodes, the specific capacity (mAh/g) is replaced by total capacity (Ah). When expressed as a fraction of the reversible capacity, the irreversible capacity has the same value regardless of the capacity units.

### 3.0 Capacity Matching

#### 3.1 Reversible Capacity

The reversible capacity represents the stable capacity that is delivered by the electrode, after the formation cycles are completed. For practical electrodes, the reversible capacity stabilizes after several formation cycles and the cumulative irreversible capacity reaches a limiting value. This is the behavior demonstrated in Figure 2. In poor-performing electrodes, the irreversible capacity may persist in prolonged cycling, leading to continued loss of cell capacity and poor cycle life. The calculations discussed in this report assume that the capacities are stable after formation.

#### 3.2 Irreversible Capacity

Irreversible capacity contributes to the total charge capacity that is absorbed by the electrode in the initial (formation) cycles. In the case of the positive electrode, the extraction of lithium in the first charge induces changes to the crystal structure, making it impossible for the same amount of lithium to be re-inserted in the subsequent discharge cycle (Ref. 3). In this case, the quantity of lithium that is removed cannot be replaced. At the negative electrode, the initial transfer of lithium reduces the potential and induces electrochemical

reactions (reduction) with the electrolyte (Ref. 4). The reduction products are electrochemically inactive species that comprise the solid electrolyte interphase (SEI). This portion of the first charge capacity cannot be accessed in discharge because the reduction products are inactive.

The cell performance forecasts presented in this report assume that the capacity performance for each electrode is the same as in half-cells. The irreversible capacity generated by each electrode must be absorbed by the opposite electrode, as lithium is transferred and current flows during the irreversible process. Allowance for the irreversible capacity forms an important consideration in the capacity balance of the electrodes in a full cell.

### 3.3 Capacity Ratio Considerations

Practical cell design requires that the capacity of the opposing electrodes be “matched”. The electrode pairs have equal active area and must exchange the same capacity in cycling. This is equivalent to completing a material balance for Li in the electrodes. The positive electrode represents the source of lithium ions for the functioning cell and there must be sufficient negative capacity to absorb the positive capacity (including positive irreversible capacity). The negative electrode is assumed to absorb the positive capacity to form the SEI layer (satisfying the negative irreversible capacity). The balance of remaining positive capacity is assumed to lithiate the negative electrode reversibly.

One of the electrodes may be designed with less capacity than the other, and will limit the capacity of the cell. In this work, calculations assume a positive-to-negative capacity ratio (P/N) that is slightly less than one, making the cell positive-limited on charge. This choice is intended to provide a slight excess of negative capacity so that lithium can be intercalated into the anode host without forming potentially hazardous (reactive) metallic lithium. In these calculations, the P/N ratio is based on the total capacity of the electrodes (irreversible plus reversible capacity).

Sample calculations for a hypothetical, positive-limited, 35 Ah cell are presented below; based on the room temperature electrode performance summarized in Figure 2.

First, assume a positive reversible capacity of 35 Ah. The positive irreversible capacity equals 19.7 percent of the reversible capacity (19.7 percent  $\times$  35 Ah = 6.90 Ah). The total positive capacity is equal to 41.90 Ah (= 35 + 6.90).

This calculation uses excess negative capacity with a P/N ratio of 0.909 (equivalent to a 10 percent excess negative capacity). Note that this is the ratio of *total* capacities, including irreversible capacity and reversible capacity. For this cell, the total negative capacity is 46.09 Ah (= 41.90/0.909).

The negative irreversible capacity is equal to 7.7 percent of the reversible capacity. Therefore, the negative reversible capacity is 42.79 Ah (= 46.09 Ah/1.077). The irreversible capacity is 3.30 Ah (=7.7 percent  $\times$  42.79 Ah). Capacity elements are summarized in Table 2 and compared side-by-side in Figure 3.

TABLE 2.—CAPACITY VALUES FOR BASELINE 35 Ah CELL

Capacity in Ah	Positive	Negative
Irreversible	6.90	3.30
Reversible	35.00	42.79
Total	41.90	46.09
Irreversible (% of rev.)	19.7%	7.7%

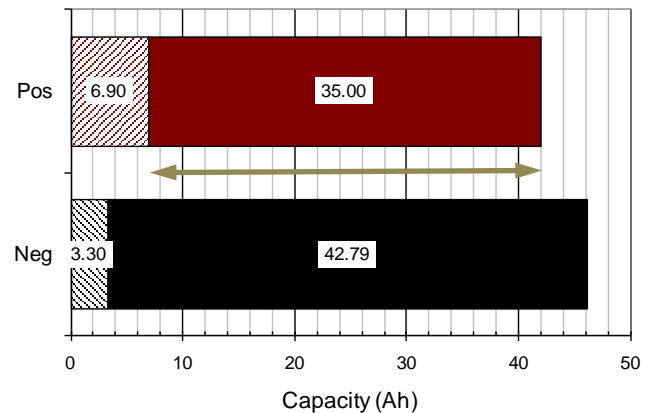


Figure 3.—Capacity Balance in a hypothetical 35 Ah cell.

This hypothetical cell has 35 Ah of reversible capacity in the positive electrode (solid region in Figure 3). Irreversible capacity is 6.90 Ah, illustrated as a hatched region in Figure 3. This positive electrode will exchange a total capacity of 41.90 Ah (irreversible + reversible capacity) with the negative electrode in order to become fully charged.

Here, the positive reversible capacity limits the useable window of operation for the negative electrode to the 35 Ah region shown by the arrow in Figure 3. The limited total positive capacity prevents the negative from becoming fully charged (as expected, since this was the intent of having excess negative capacity). In addition, due to the balance of irreversible capacities, the negative electrode cannot be discharged past the left of the arrow because of the lower limit of positive capacity.

Thus, the maximum state-of-charge for the anode is 90.2 percent:

$$(6.90 + 35 - 3.30)/42.79 = 90.2\%$$

The minimum state-of-charge for the anode is 8.4 percent:

$$(6.90 - 3.30)/42.79 = 8.4\%$$

The required weight of electrode active material is computed using the reversible specific capacity for the electrodes given in Table 1 and the total capacity derived in. Results of this calculation appear in Table 3.



TABLE 3.—ELECTRODE ACTIVE MATERIAL CALCULATION

	Positive	Negative
Reversible capacity (Ah)	35.00	42.79
Specific capacity (mAh/g)	152.85	334.50
Active material (g)	229.0	127.9

With the mass of electrode materials established, the voltage of the electrodes (data from Figure 2) can be determined as a function of the common total capacity as shown in Figure 4.

## 4.0 Discharge Performance Estimation

Here, the process for forecasting cell discharge voltage is described. Laboratory data for single electrodes in half-cells, with lithium metal, is used to predict cell voltage. As seen in Figure 4, the positive-limited capacity restricts the useful voltage window of the negative electrode. The negative electrode in this example will experience the voltage history illustrated by the solid black line in Figure 4. The inaccessible negative capacity (illustrated by dotted lines) cannot be utilized. This comparison illustrates how the irreversible capacity and P/N ratio affects the maximum utilization of the individual electrodes. The arrow in Figure 4 indicates the 35 Ah window for cycling capacity. The limits for the negative electrode state-of-charge in cycling were calculated above to be between 8.4 and 90.2 percent of the reversible negative capacity.

### 4.1 First Charge Capacity

The first charge capacity accounts for the irreversible capacity of both electrodes. Depending on the P/N ratio, only a portion of the total electrode capacity of the non-limiting electrode can be accessed. The P/N ratio and the balance of the irreversible capacity of the electrodes dictate the useful state-of-charge window of the electrodes. In most cases, this means that the electrodes will not see the full voltage range that was used for half-cell testing. This is illustrated for the negative electrode in Figure 4. In the initial charge, the total capacity of the positive electrode (41.9 Ah) limits the state-of-charge of the negative to 90.2 percent of its reversible capacity. When the positive electrode is fully discharged, 8.4 percent of the total negative discharge capacity remains.

Once the state-of-charge window for both electrodes is determined (by the material balance described above) the discharge voltage for the full cell can be estimated.

### 4.2 Discharge Capacity at Room Temperature

In this example, the reversible positive electrode capacity is fully utilized on discharge, delivering 35 Ah between electrode potential limits of 4.2 to 3 V vs. Li/Li<sup>+</sup>. Only a portion of the reversible negative capacity is accessed (as discussed above) with state-of-charge ranging from 8.4 to 90.2 percent.

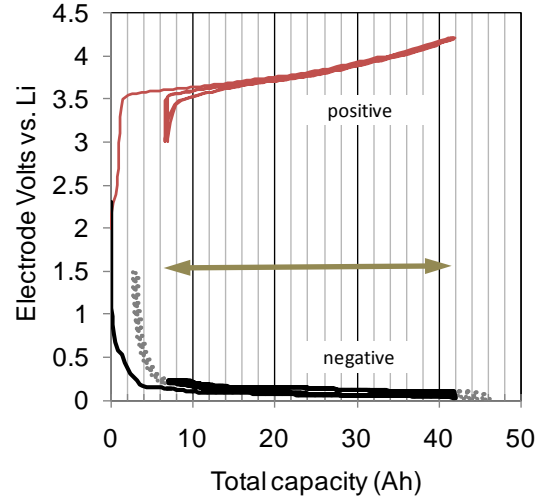
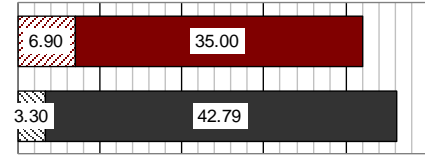


Figure 4.—Electrode voltage profiles in 35 Ah cell.

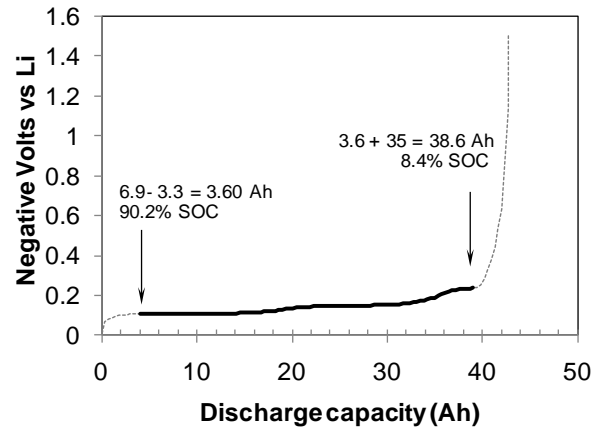


Figure 5.—Discharge capacity window for the anode.

This 35 Ah portion of negative capacity is illustrated by the solid black line in Figure 5: now plotted as *discharge* capacity. The negative electrode has a relatively flat voltage profile in this limited window of operation (0.1 to 0.24 V vs. Li/Li<sup>+</sup>).

Finally, cell voltage is calculated as the difference between electrode potentials (positive minus negative) over the selected capacity range. Discharge capacity profiles for the the electrodes and cell appear in Figure 6. For this example, the positive electrode capacity was selected to deliver 35 Ah, based on a positive electrode cutoff voltage of 3 V vs. Li/Li<sup>+</sup>. Factoring in the effect of the negative electrode, the projected cell voltage reaches a 3 V cutoff at only 34.3 Ah, 98 percent of the 35 Ah target capacity.

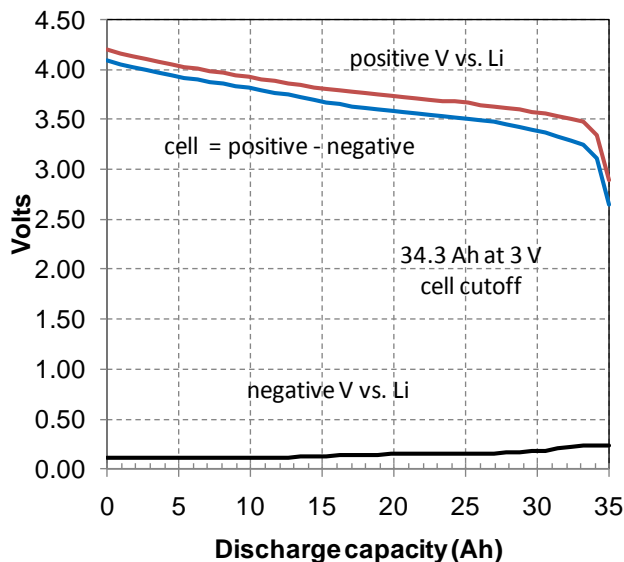


Figure 6.—Electrode and cell potential for the 35 Ah cell.

In practice, the electrode capacity is determined by trial-and-error in order to satisfy the goals for cell-level capacity at specified cut-off voltages. The spreadsheet model used to forecast cell discharge performance automates the calculations described above. Analogous calculations can be made for any combination of electrodes. For the experimental electrodes presented in this report, positive capacity has to be increased to 35.75 Ah to achieve 35 Ah at the cell level with a 3 V cutoff voltage.

### 4.3 Electrode Loading and Composition

Electrode loading refers to the mass of electrode material per unit electrode area. It is an important parameter in cell design. At constant capacity, increased loadings (thicker mix layers) offer a reduction in total electrode area and reduce the cell mass due to a savings in current collector and separator material. There is a trade-off however, since increased loadings tend to diminish the utilization of the electrode material, effectively reducing the specific capacity. Electrode loading was not dictated in the original list of key performance parameters (KPPs) for electrodes.

In performing cell-level estimates, capacity balance is established as outlined in the sample calculations above. Electrode area is then adjusted to produce the desired loading. The electrode area in the above example is 12,100 cm<sup>2</sup>, with a corresponding loading of 2.9 mAh/cm<sup>2</sup>. The positive electrode mass loading 22 mg/cm<sup>2</sup>, including active material and all electrode additives. The negative electrode mass loading is projected to be 11 mg/cm<sup>2</sup>. The electrode layer that is deposited on the current collector foil is estimated to be 80 μm in thickness for both electrodes. Electrode composition (binder and conductive diluent level) also impact the discharge performance (rate capability) and total electrode mass.

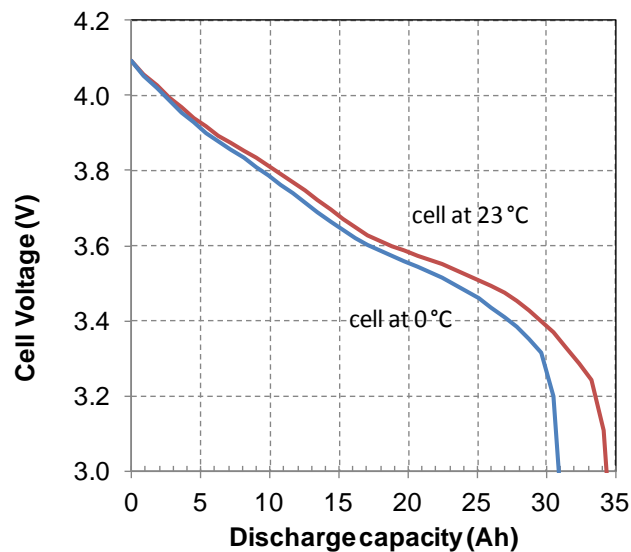


Figure 7.—Projected cell capacity at 0 °C.

### 4.4 Rate Capability and Temperature Effects

The example calculations above are based on electrode data collected at room temperature and C/10 rates. However, the ETDK KPP for capacity was originally specified for discharge at 0 °C. At reduced temperature (or higher discharge rates); the cell voltage reaches the cut-off value at a lower discharge capacity. Temperature and rate effects are captured in the model by substituting single-electrode data collected under the alternative conditions.

Discharge performance for this cell was estimated by assuming a 10 percent loss in cathode capacity at 0 °C. The reduced positive electrode performance results in a projected cell capacity of 31 Ah at the 3 V cutoff (see Figure 7). In order to meet the KPP goal of 35 Ah at 0 °C, the hypothetical cell discussed here would have to be sized for additional capacity.

### 4.5 Cell-Level Energy Calculation

Cell discharge energy is calculated by integrating cell discharge voltage over the discharge capacity. This is done numerically in the spreadsheet model. This 35 Ah example cell delivers 125 Wh at a cell cutoff voltage of 3 V.

Cell mass is calculated with high fidelity by the model and includes, all electrode materials, electrolyte, foils, internal tabbing connections and terminals. The case material is computed to enclose the electrode package with allowance for header space and lateral clearance between the inner case wall and the edges of the electrodes. The 35 Ah cell presented here is estimated to have a mass of 0.72 kg, distributed as shown in Table 4.

The projected specific energy for this cell is 174 Wh/kg at room temperature. The projected specific energy at 0 °C is 157 Wh/kg, 90 percent of the room temperature value.

TABLE 4.—ESTIMATED CELL MATERIAL MASS IN GRAMS

Electrochemical	628.3	87.3%
Enclosure materials	48.1	6.7%
Terminals/edge material	2.9	0.4%
Header	40.5	5.6%
Total cell	719.8 grams	

Using this model, it is projected that that target capacity of 35 Ah at 0 °C could be achieved by a cell with a room temperature capacity of approximately 40 Ah. Such a cell would have a specific energy of 159 Wh/kg at 0 °C.

## 5.0 Discussion

The calculation procedures described above provide a means for projecting cell-level specific energy based on laboratory data for the individual electrodes. These estimates capture the effect of irreversible capacity, reversible capacity and P/N ratio. Results are based on test data for real electrodes in half-cells. The accuracy of such projections depends heavily on the assumptions for electrode makeup. In particular, changes in porosity and electrode loading will have a significant effect on the rate capability of the electrode. In performing estimates, data at specific loadings and electrode porosity was available.

It has already been pointed out that the capacity balance will restrict the allowable capacity window of the electrode with

excess capacity (the negative electrode in the examples above). In turn, the model assumes that the electrode voltage/capacity behavior of the affected electrode is the same as if the electrode was fully formed. The portability of the half-cell data, with full state-of-charge, to the model with partial formation and state of charge represents a large assumption in this work and should be verified experimentally.

It should be underscored that these estimates represent the initial capacity and energy of the cell. Deterioration of performance with cycle life is not captured in these estimates.

The half-cells used to collect data for the single electrodes includes ohmic drop for *one* layer of separator material. Forecasts for cell voltage are derived by difference between the electrode potentials and as such, it includes the ohmic loss of two separators. This small error has been neglected in making cell-level estimates.

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