Glenn Research Center

Considerations for Estimating Electrode Performance in Li-Ion Cells

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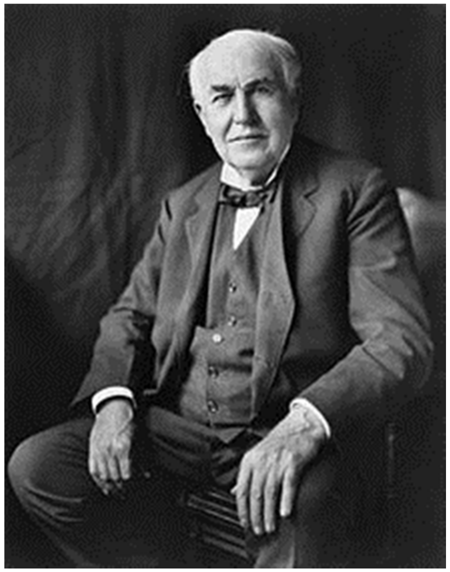
Performance estimation

"The storage battery is one of those peculiar things which appeals to the imagination, and no more perfect thing could be desired by stock swindlers than that very selfsame thing.

Just as soon as a man gets working on the secondary battery it brings out his latent capacity for lying."



Thomas Edison
Harper's Monthly (1932)

We want to make realistic predictions for battery performance

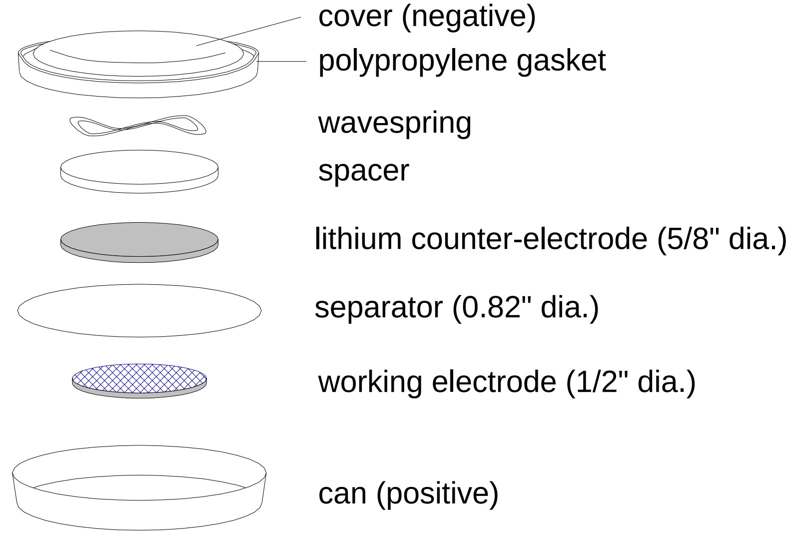
Li-ion Cell Performance Projections

- Testing of individual electrodes
  - Reversible capacity
  - Irreversible capacity
- Matching electrodes in full cells
- Cell performance estimation – Wh/kg

How does electrode performance relate to cell performance?

Half-cell testing

- Working electrode vs. lithium metal
- Excess negative capacity (> 30x)
- Lithium counter-electrode serves as a pseudo-reference electrode
- Provides data for working electrode capacity and voltage performance



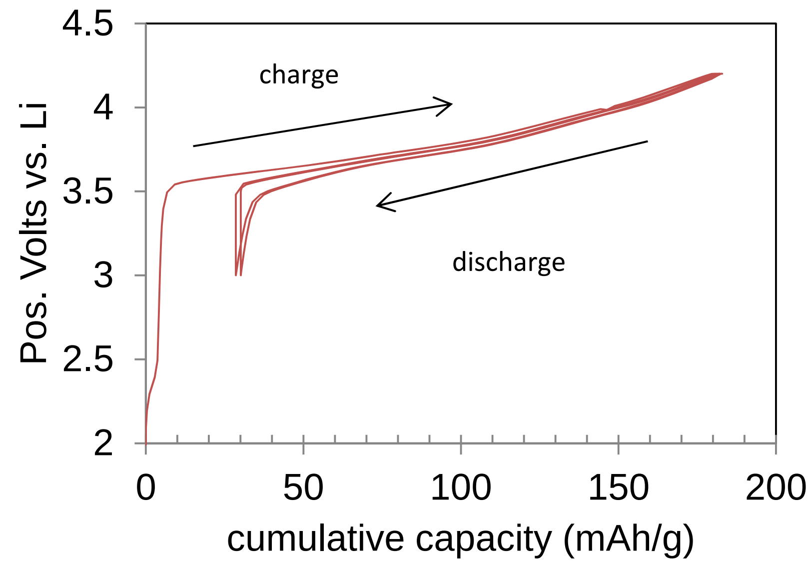
Half-cell testing – Positive electrode

- Cycled to voltage limits

  Upper limit: 4.2 V vs. Li

  Lower limit: 3.0 V vs. Li

- Capacity per gram of *active* material in the positive electrode
- Cumulative capacity, running total of charge - discharge
- Data for first three cycles at C/20



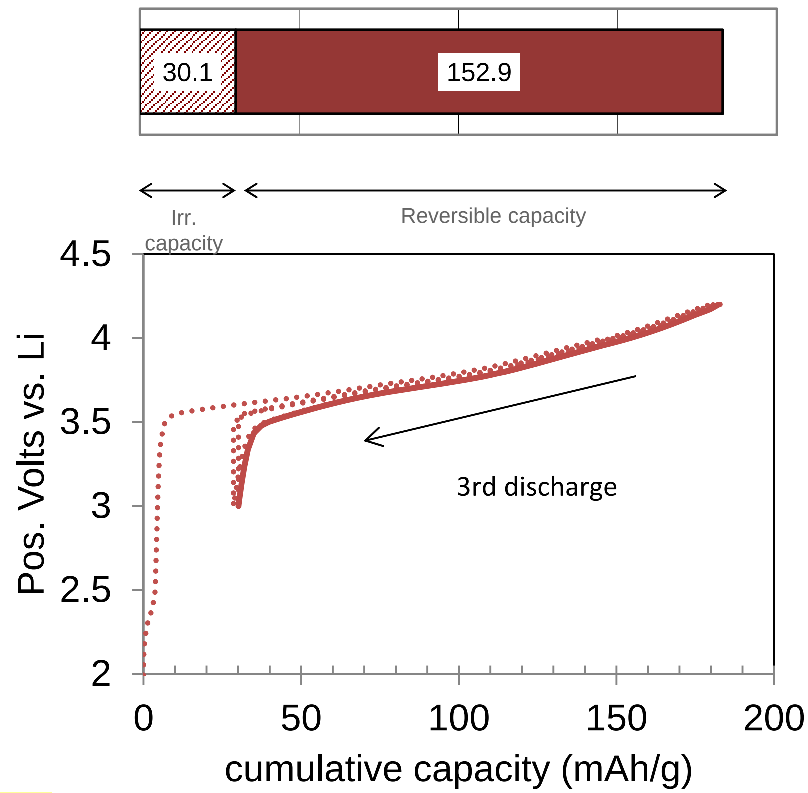
Half-cell testing – Positive electrode

- After three cycles:

  153 mAh/g reversible capacity

  30 mAh/g irreversible capacity

  183 mAh/g total capacity



Based on positive material alone:

153 Ah/kg x 3.7 $V_{avg.}$ = 566 Wh/kg

Half-cell testing – Negative electrode

- Cycled to voltage limits

  Lower limit: 10 mV vs. Li

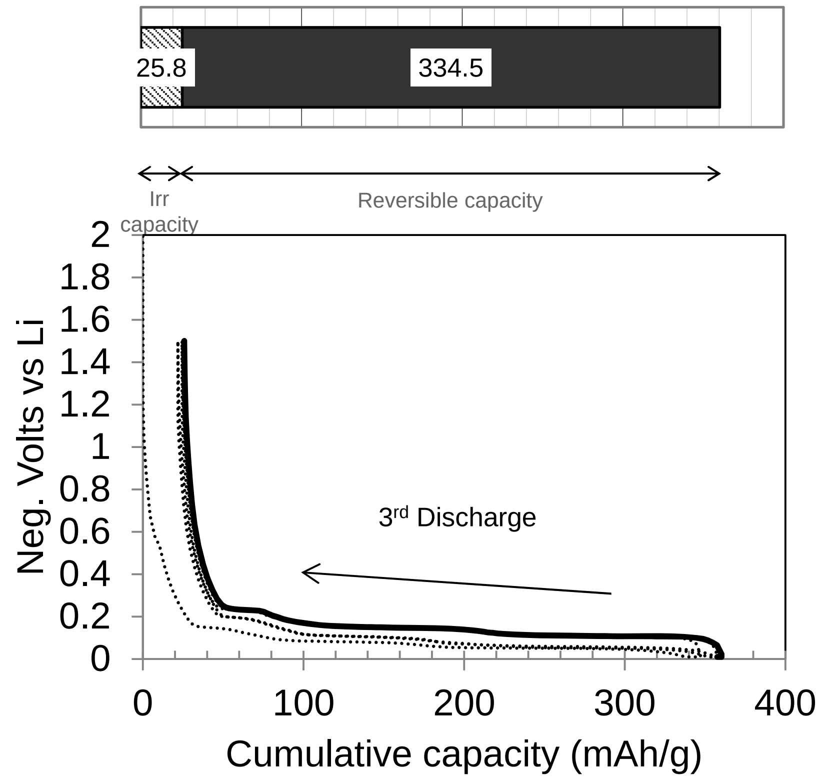
  Upper limit: 1.5 V vs. Li

- Capacity per gram of *active* material in negative electrode
- After three cycles at C/20

  334 mAh/g reversible capacity

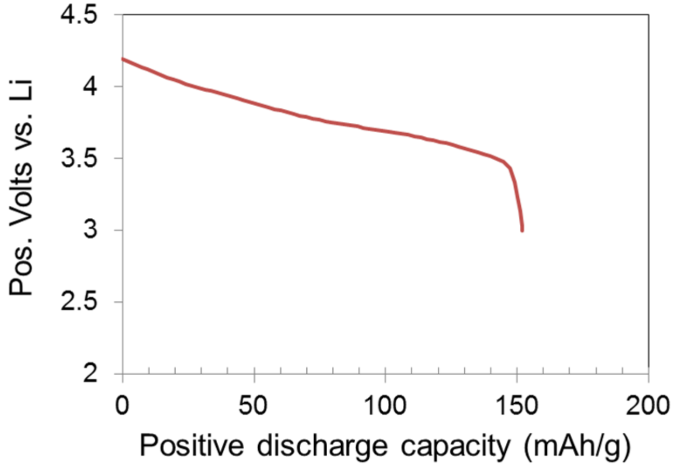
  26 mAh/g irreversible capacity

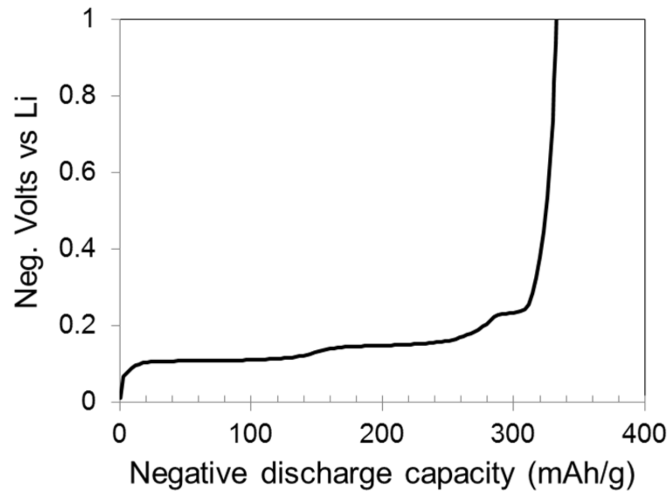
  360 mAh/g total capacity



Electrode Capacity Summary

Capacity in mAh/g	positive	negative
Irreversible capacity	30.1	25.8
Reversible capacity	153.9	334.5
total	183.0	360.3
irreversible capacity as a fraction of reversible	19.7%	7.7%





Let's design a 35 Ah cell using these electrodes.

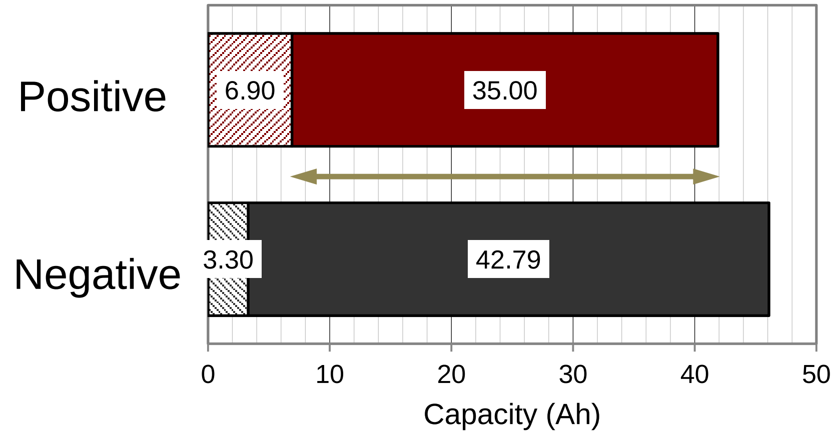
Design of a 35 Ah Cell

- Choose 35 Ah of reversible positive capacity
- 41.9 Ah of *total* positive capacity must be accepted by the negative
- Allow 10% excess *total* negative capacity:

  110% x 41.9 = 46.09 Ah

  P/N = 0.909
- Negative is not fully utilized

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%



Calculations assume same irreversible capacity as in half-cells

Design of a 35 Ah Cell

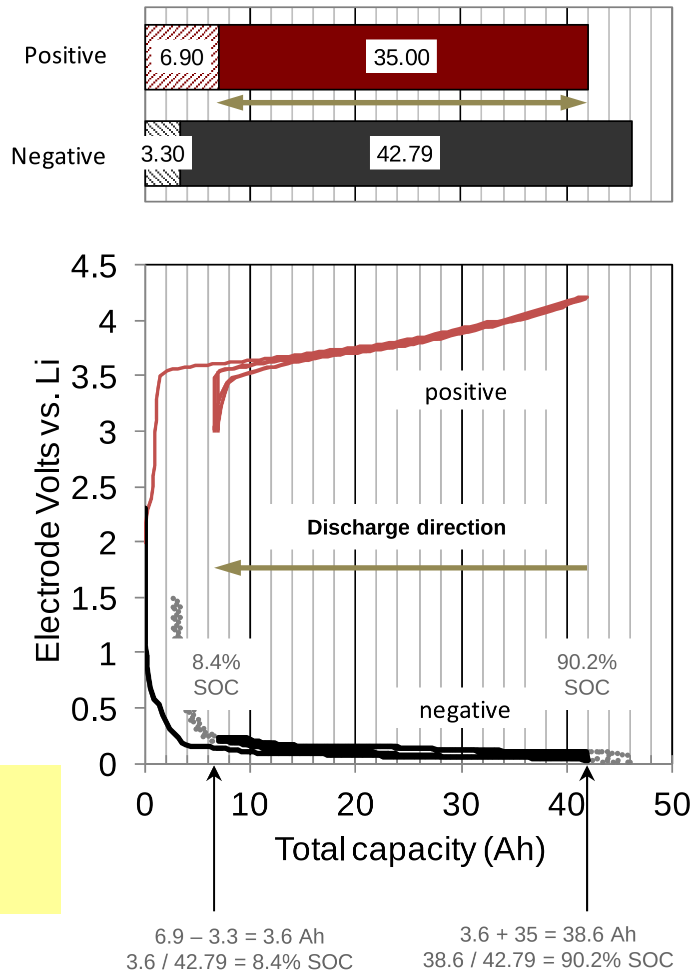
<u>Negative electrode utilization</u>

- State-of-charge window for the negative electrode:

  90.2% to 8.4% SOC

- Positive capacity is fully utilized

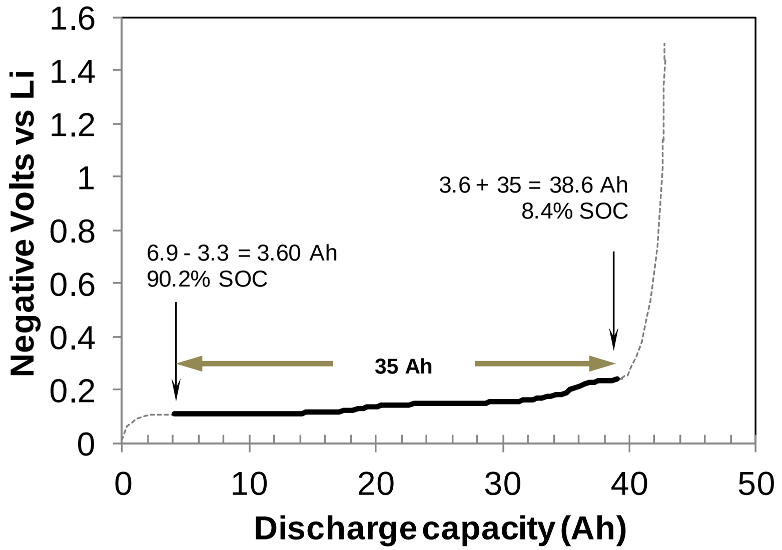
Assumes positive irreversible capacity charges the negative to 8.4% SOC



Prediction of Cell Discharge Voltage

Negative electrode

- Assume negative voltage performance as in half-cell
- Delivers 35 Ah between 90.2% to 8.4% SOC
- Projected discharge voltage in bold

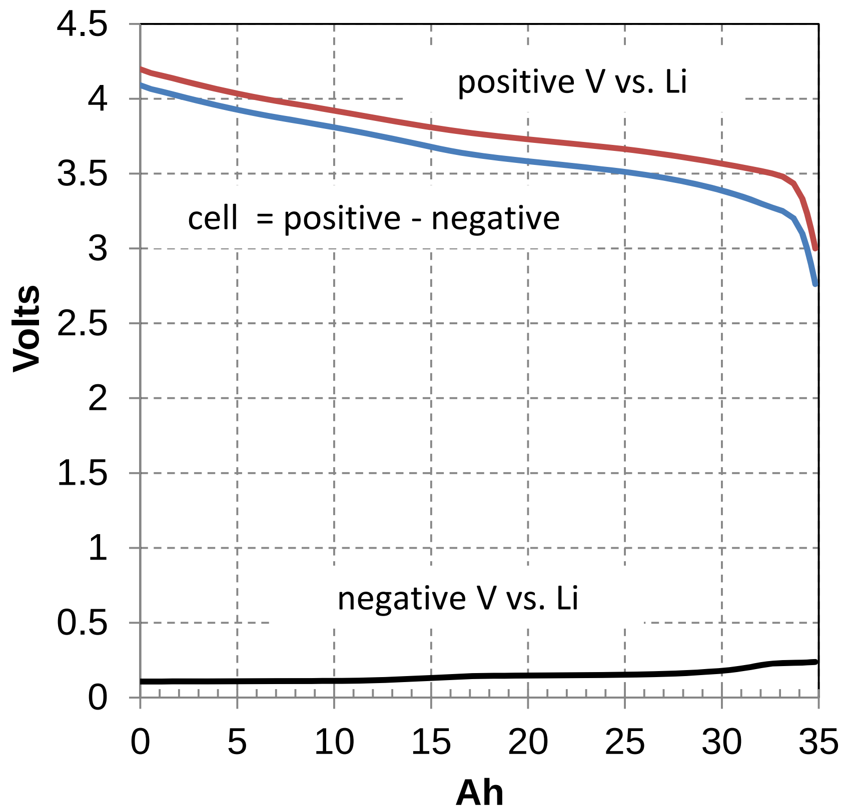


Assumes the partially charged negative has discharge voltage similar to fully charged negative in half-cell.

Prediction of Cell Discharge Voltage

<u>Combined electrode voltage</u>

- Full utilization of positive
- Limited utilization of negative
- Cell voltage by difference
- Projection for low rate (C/20)

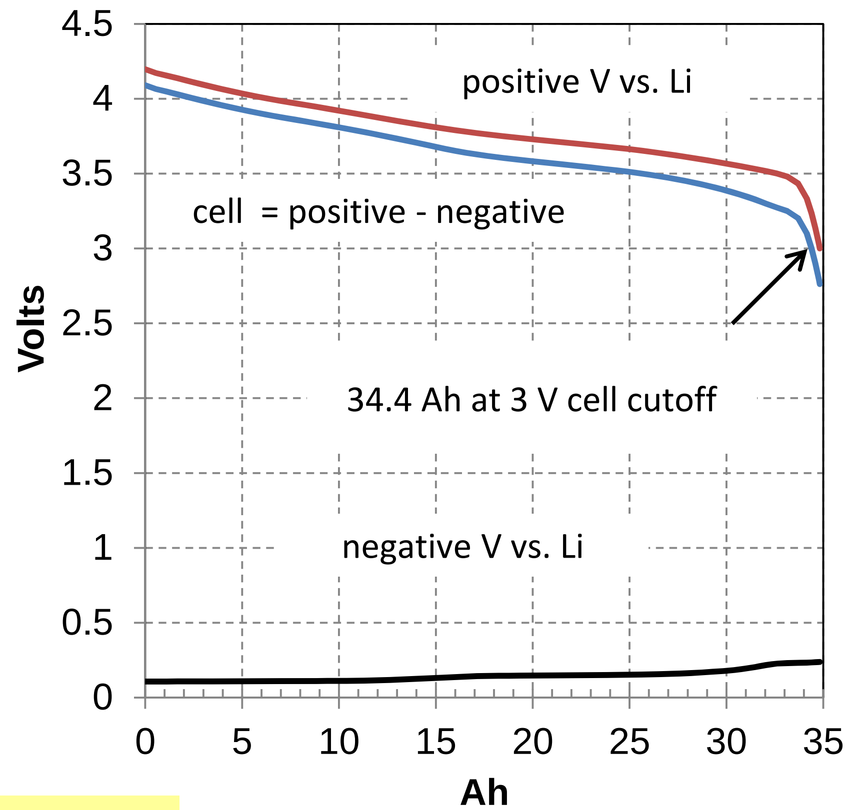


Not applicable to higher discharge rates

Prediction of Cell Discharge Voltage

<u>Projected cell capacity</u>

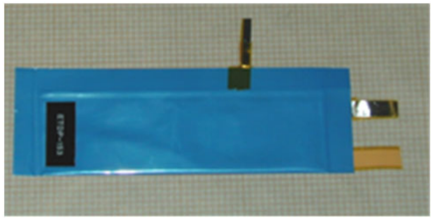
- Choose 3 V cut-off for cell discharge voltage
- ~34.4 Ah cell capacity

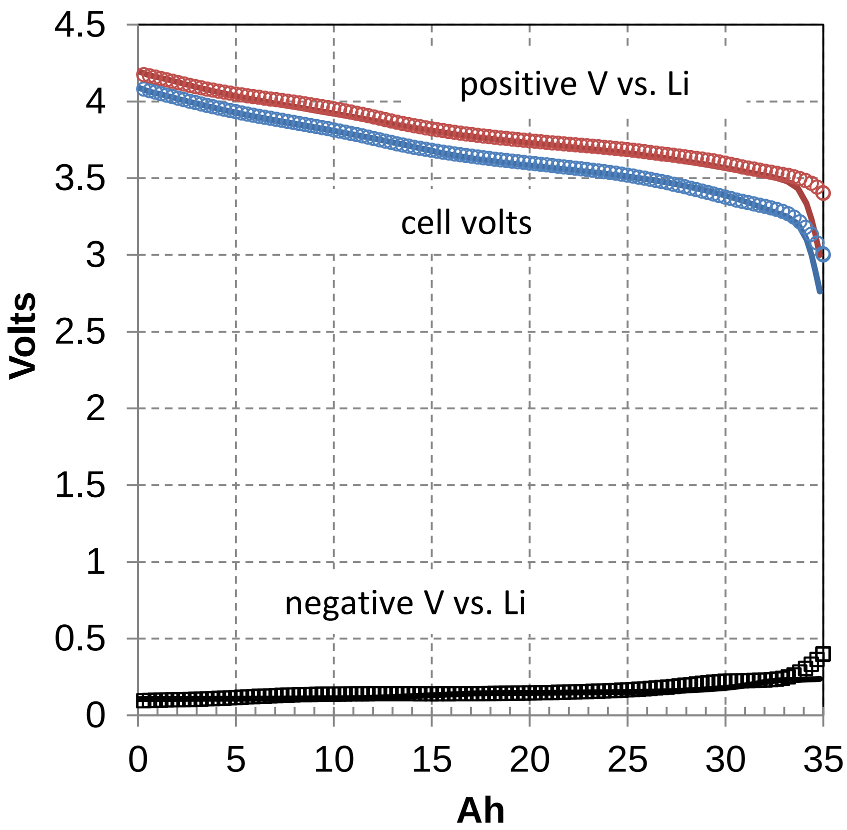


Cell voltage cutoff limits full utilization of the positive electrode capacity

Voltage projection vs. full cell data

- Pouch cell with reference electrode, built using same materials as half-cells.
- Reasonable match between data (open symbols) and projections.

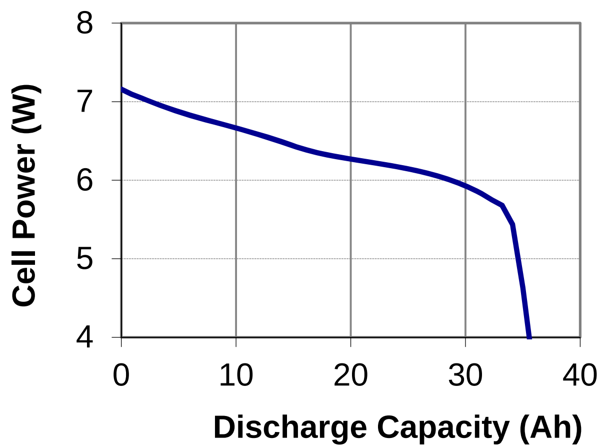


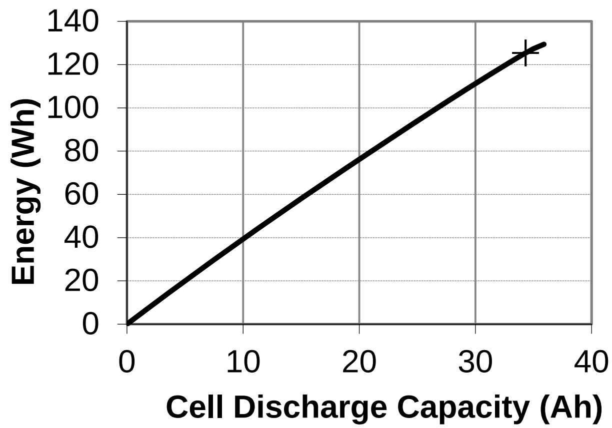


Discharge Energy Projection

Electrical energy:

- Calculate power at given current using projected cell voltage
- Integrate power to estimate energy delivered
- 125 Wh at 3 V cutoff





Projected for low discharge rate (C/20 = 1.75 A)

Cell Mass Projection

Cell mass:

- Electrodes = 0.40 kg
- Total material (including electrolyte, separator, current collector) = 0.56 kg
- Allow 18% additional mass for cell case material
- Finished cell = 0.66 kg

	positive	negative
Reversible capacity (Ah)	35.00	42.79
Specific capacity (Ah/kg)	153.9	334.5
Active material (kg)	0.227	0.127
Active material fraction	86%	97%
Total Electrode (kg)	0.27	0.13

Electrodes represent ~60% of the finished cell mass

Specific Energy Projection

Cell-level estimate:

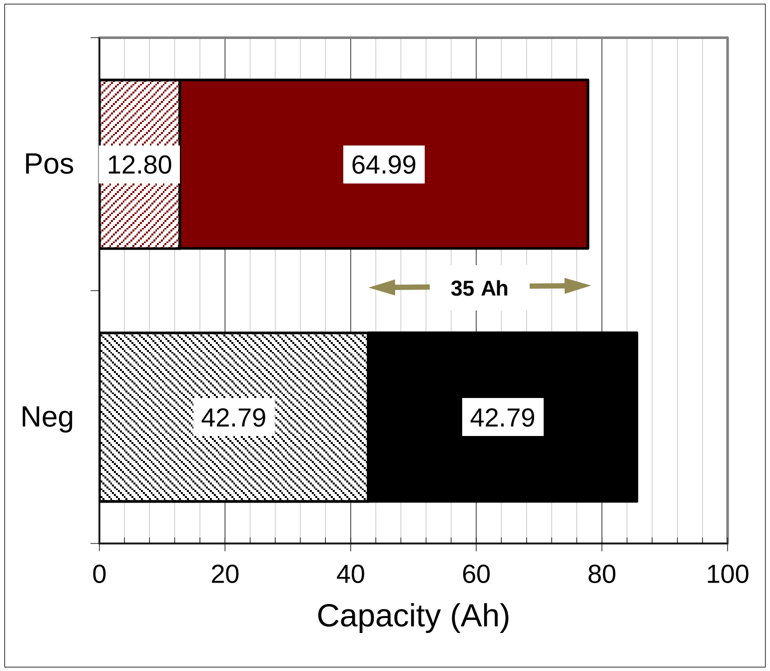
- Energy at C/20 rate to 3 V = 125 Wh
- Finished cell mass = 0.66 kg
- Projected specific energy = 189 Wh/kg

Estimate for a single cell.
Battery-level specific energy would be less!

Effect of High Irreversible Capacity

35 Ah cell with same positive material.

- 1000 mAh/g negative reversible
- 100% irreversible
- Projected energy = 154 Wh/kg



Un-utilized positive capacity adds significant mass to cell.
Erases the benefit to of high negative specific capacity.

Summary

What was shown:

- Capacity considerations (irreversible, reversible, P/N ratio)
- A method to project cell discharge voltage using data for individual electrodes
- Specific energy estimation

Estimates at other rates and temperatures would require half-cell data at the relevant conditions

Acknowledgement

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Carolyn Mercer, PhD.

Project Manager

NASA Glenn Research Center

Thank You