Design and Simulation of Spirally-Wound, Lithium-Ion Cells

Article *in* ECS Transactions · July 2013

DOI: 10.1149/05026.0209ecst

11 authors, including:

Robert Spotnitz
Battery Design LLC
46 PUBLICATIONS **2,695** CITATIONS
SEE PROFILE

Steve Hartridge
6 PUBLICATIONS **19** CITATIONS
SEE PROFILE

Gaetan Damblanc
CD-adapco
4 PUBLICATIONS **169** CITATIONS
SEE PROFILE

Christopher Lueth
Siemens
14 PUBLICATIONS **63** CITATIONS
SEE PROFILE

Design and Simulation of Spirally-Wound, Lithium-Ion Cells

R. Spotnitz[a], S. Hartridge[b], G. Damblanc[b], G. Yeduvaka[b], D. Schad[b], V. Gudimetla[b], J. Votteler[b], G. Poole[b], C. Lueth[b], C. Walchshofer[b], and E. Oxenham[b]

[a]Battery Design LLC, 2277 Delucchi Drive, Pleasanton, CA 94588
[b]CD-adapco, 60 Broadhollow Road, Melville, NY 11747

A general approach for the design of cylindrical and prismatic spirally-wound lithium-ion cells that accounts for arbitrary tabbing and coating patterns is presented. Examples are presented for design of high-power and high-energy 18650 size cells. For high-energy cells the current collector design is not critical while for high-power cells the tabbing design is significant especially when thermal effects are considered.

Introduction

The spirally-wound format is the most common design of lithium-ion cells. Lithium-ion cells are usually made with very flexible, thin electrodes (each typically less than 250 microns thick) and separators (typically less than 30 microns thick), so winding these layers around a mandrel (either cylindrical or prismatic) is not only possible, but very amenable to high-speed production. Despite the widespread popularity of the spiral-wound design, software for the analysis and design of these cells is limited because of the complexity of modeling the spiral geometry and difficulties in accounting for the myriad possibilities of electrode designs which have different tabbing and coating patterns. This paper describes a general approach for design and simulation of spirally-wound, lithium-ion cells.

Approach

Reimers (1) provides a good introduction to the problem of designing spirally-wound cells. Here Reimers' approach is extended to consider the effects of tab width, tab overlap with current collector foil, uncoated sections of electrode, and electrode height. Inclusion of these effects can greatly increase the number of nodes required in the numerical solution and so the computational expense. The problem can be appreciated by considering a spiral discretized by evenly spaced circumferential lines (see Figure 1).

Discretizing the spiral as in Figure 1 insures that the electrochemical cells formed by opposing electrodes, called "ecells" for brevity, are well defined as long as electrodes start and end at one of the circumferential lines. The number of ecells could be significantly reduced by merging circumferential segments. For example, referring to Figure 2, the black electrode is divided into segments $0\rightarrow1$, $1\rightarrow2$, $2\rightarrow3$, $3\rightarrow4$ $4\rightarrow5$, $5\rightarrow6$. The "ecells" are defined where the black segment faces a grey segment (the white segments represent separators). The segment $0\rightarrow1$ defines an ecell on the outer surface

of the black electrode. Segment 1→2 defines ecells on the inner and outer surfaces; however the inner segment is poorly defined because part of the segment does not face the grey counter electrode. This demonstrates that an arbitrary, non-uniform spacing is not possible.

The problem illustrated in Figure 2 can be overcome by adding nodes at the start and end of each electrode (see Figure 3). More generally this approach can be used to resolve features such as tabs and uncoated sections of electrode.

However, the grid illustrated in Figure 3 is still not well defined because the inner ecell defined by segment 3→4 conflicts with the outer ecell defined by segment 1→2. To overcome this problem, separate grids can be used for the two electrodes, and interpolation used to map points between grids.

Note that while the potential distribution, found by solving Poisson's equation, needs to be computed for both the positive and negative current collectors, the current flowing between electrodes, found by solving an electrochemical cell model, for both inner and outer ecells need only be solved for one grid, and interpolation can be used to compute ecell currents for the opposite grid.

The current flow between electrodes can be found as function of the potential difference between the plates using an electrochemical cell model. For the examples here, a state-of-charge dependent resistor model similar to that Kim et al. (2) is used, though alternative models such as the DUALFOIL type (3-4) can be used.

This approach enables complex electrode designs to be analyzed with minimal computational effort. The grid can readily be extended to cover the width of the electrodes. The use of Poisson's equation to solve for potential distribution along the circumferential path of both electrodes, and an electrochemical cell model to solve for the current flowing between electrodes completely defines the electrical problem. The coupled thermal problem also needs to be addressed.

The simplest approach for coupling the thermal problem is to use a lumped energy balance, so the entire cell heats and cools uniformly, to solve for the temperature. The energy balance computes a temperature using a heat generation term that is computed from the solution of the electrical model, and provides that temperature to the electrical model. Alternatively, a thermal grid can be defined which is mapped to the electrical grid. In this case, the thermal solver takes heat generation terms from the electrical solution and provides temperature values to the electrical solver. For the examples here, a lumped energy balance is used.

The above approach has been implemented in the Battery Design Studio® (BDS) software (see http://www.cd-adapco.com/products/battery_design_studio/). The software provides for user-friendly selection of different electrode designs and automatic generation of a spiral.

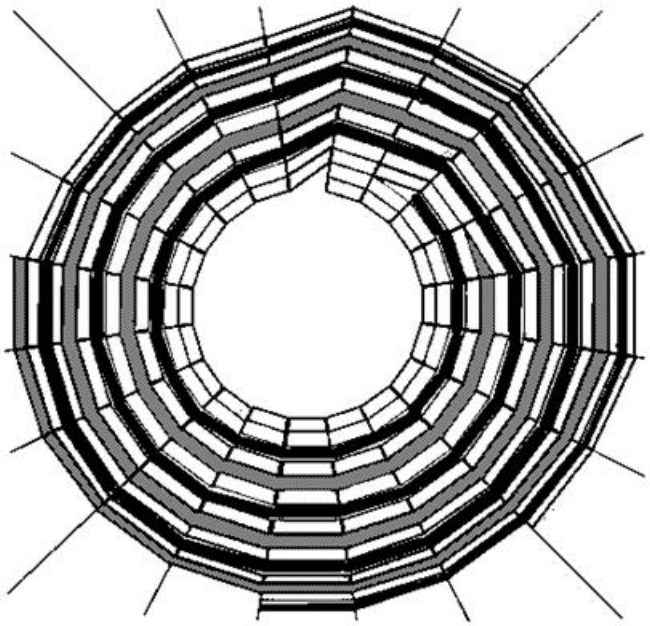

Figure 1. Top view of spirally-wound cell discretized by evenly-spaced, circumferential lines. Black and grey curves indicate electrodes (of opposite polarity) and the white spaces indicate separators.

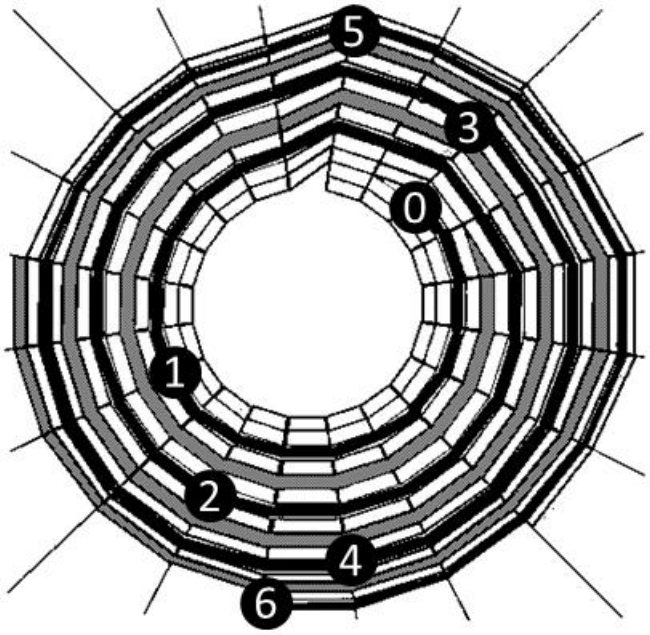

Figure 2. Top view of spirally-wound cell with non-uniform spaced segments defined by numbered nodes.

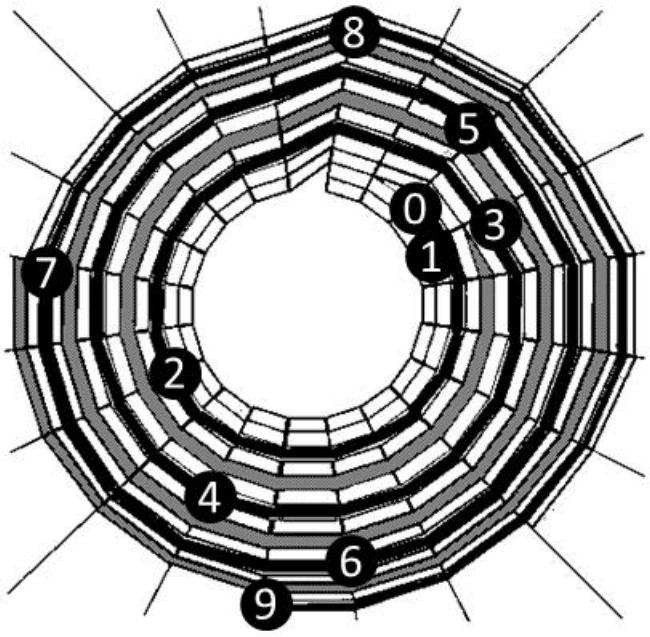

Figure 3. Top view of spirally-wound cell with non-uniform spaced segments that includes nodes at beginning and end of each electrode..

Examples

The single most popular lithium-ion cell design is the 18650. This is a cylindrical cell approximately 65 mm tall and 18 mm in diameter typically with the negative tab connected to the bottom of the can and the positive tab to the header. 18650 cells are available in a variety of chemistries and cell capacities, but can generally be classified as high-power or high-energy cells. Here examples of both types are considered.

Both a high energy and high power 18650-size cell were designed in BDS. A 1-dimensional DUAL type model (3-4) was used to generate synthetic voltage curves at different rates. This synthetic data was fit to a simple resistance model (called NTGP to honor the contributors J. Newman, W. Tiedemann, H. Gu, and W. Peukert) similar to that of Kim et al. (2), and then used to carry out simulations using the approach described above (see Figure 4).

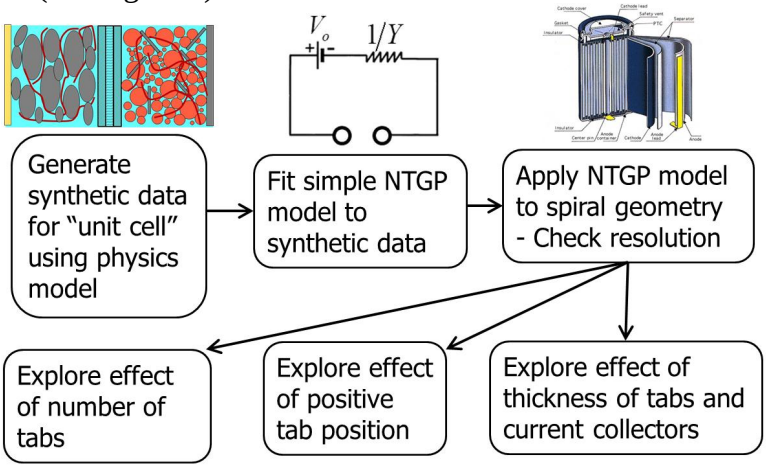

Figure 4. Analysis approach for high-power cells.

High Energy Cell. Several high energy cell designs with different current collector thickness values were designed using a LiNiCoAlO2/graphite chemistry. The ratio of current collector thickness was selected so that the linear resistances of the positive and negative collector would be nearly equal. Increasing the current collector thickness decreased the resistance of the collectors and resulted in a slight decrease in cell capacity (see Table 1). The reduction in ohmic voltage drop at the relatively high current of 6.8 A is only 22 mV when the positive collector is increased from 20 to 26 microns while the capacity is decreased by 0.08 Ah. Since high energy cells are typically operated at lower currents (0.2 C-rate to 0.5 C-rate), the ohmic drop along the lengths of the electrodes is relatively small and there is little benefit to increasing current collector thickness.

TABLE I. Effect of collector thickness on capacity an ohmic drop for high energy cell.

Collector thickness, mm		Cell, Ah	Ohmic Drop @ 6.8 A, ,mV
Positive	**Negative**		
13	8	2.99	142
20	12	2.89	93
26	16	2.81	71

High Power Cell. A NCM/graphite chemistry was used; some of the electrode properties are summarized in Figure 5. The results from the discharge simulations using the 1-dimensional physics-based model are presented in Figure 6.

Computed Electrode Properties	Positive Value	Negative Value
Average Voltage, V	3.87	0.133
Stoichiometry at formation	0.450	0.905
Unit Capacity*, mAh/cm²	1.775	1.812
Thickness(w/collector), µ	116.000	108.000
Coating Porosity, %	40.0	40.0
Coated Length*, cm	170.353	170.953
Coating Thickness*, µ	50.000	48.000
Coating Weight, g	12.379	6.217
Total Length, cm	88.627	90.727
Loading, mg/cm²	24.927	12.265

Figure 5. Screenshot from BDS showing selected properties of electrodes for high-power design.

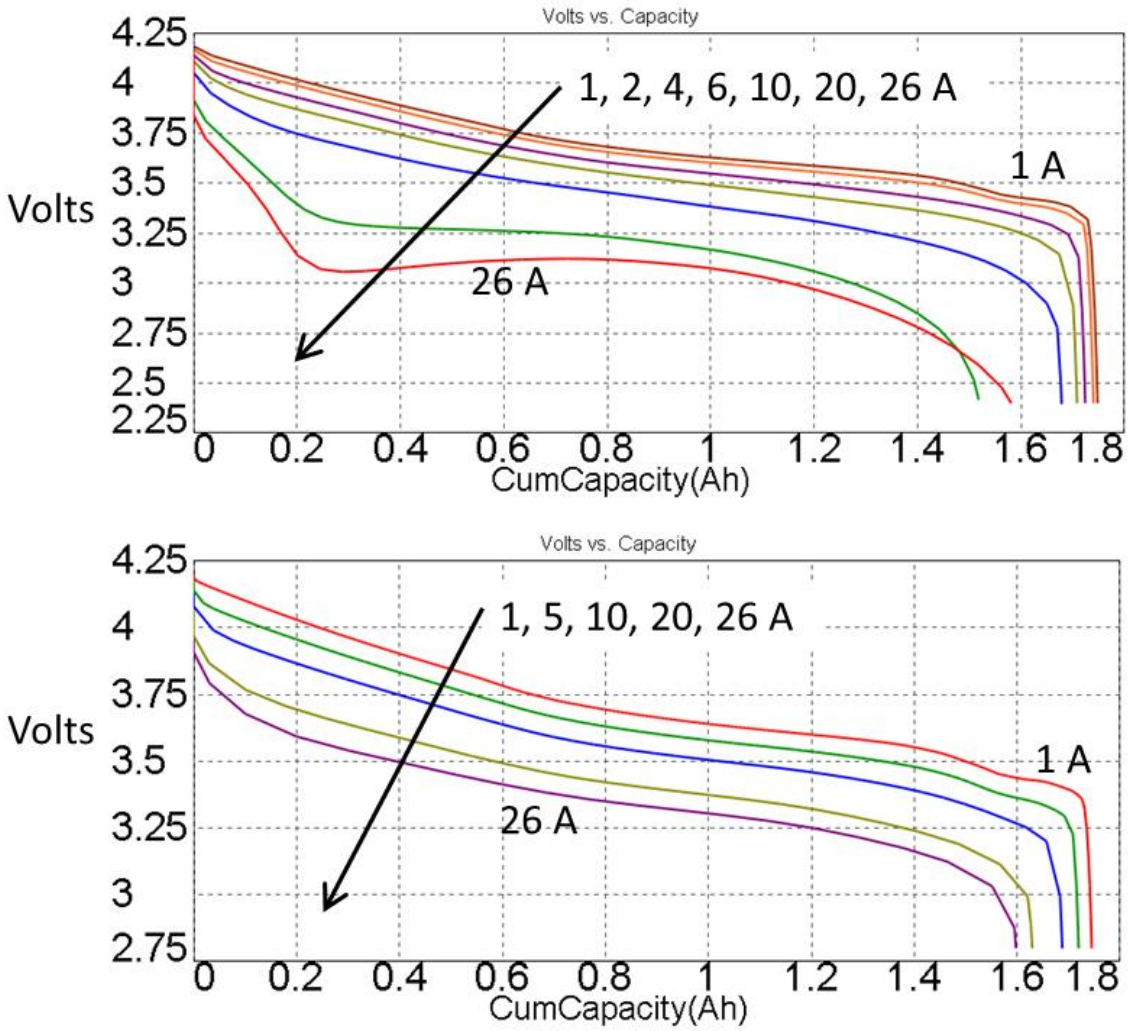

Figure 6. Simulated discharge curves for high power cell using 1-dimensional DUAL model (called DISTNP in BDS).

<u>High Power Cell: Opposite versus Same Side Tabs.</u> In this cell design the positive and negative electrodes each have a single tab at one end (see Figure 7) and are wound so that the positive tab is at the center of the spiral and the negative tab is at the outer radius of the spiral, or both tabs are at the center of the spiral.

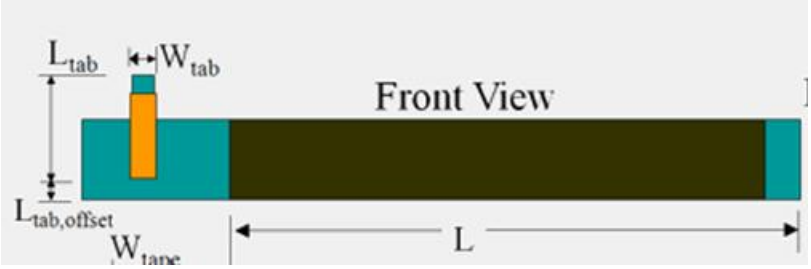

Figure 7. Screenshot from BDS showing single tab electrode design.

Positioning the tabs at opposite ends provides a more uniform state of charge distribution in the cell which enables more capacity to be extracted (see Figure 8). Given that the

opposite ends design is preferred, the effect of collector thickness can be examined. As before, the thickness of the negative collector is adjusted so that the linear resistances of the positive and negative collectors are nearly the same. For the high power cell design with tabs at opposite ends, there is an optimum positive collector thickness at 20 microns (see Figure 9).

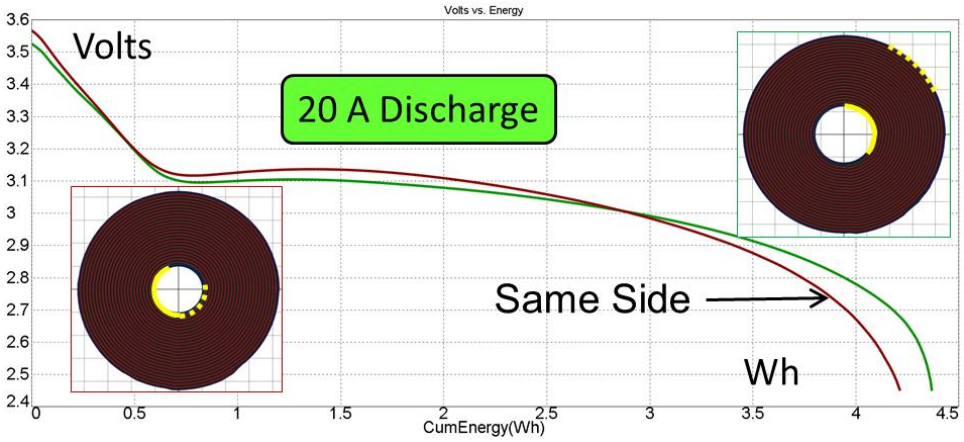

Figure 8. Simulated discharge curves for 18650 cells with tabs on same ends and tabs on opposite ends.

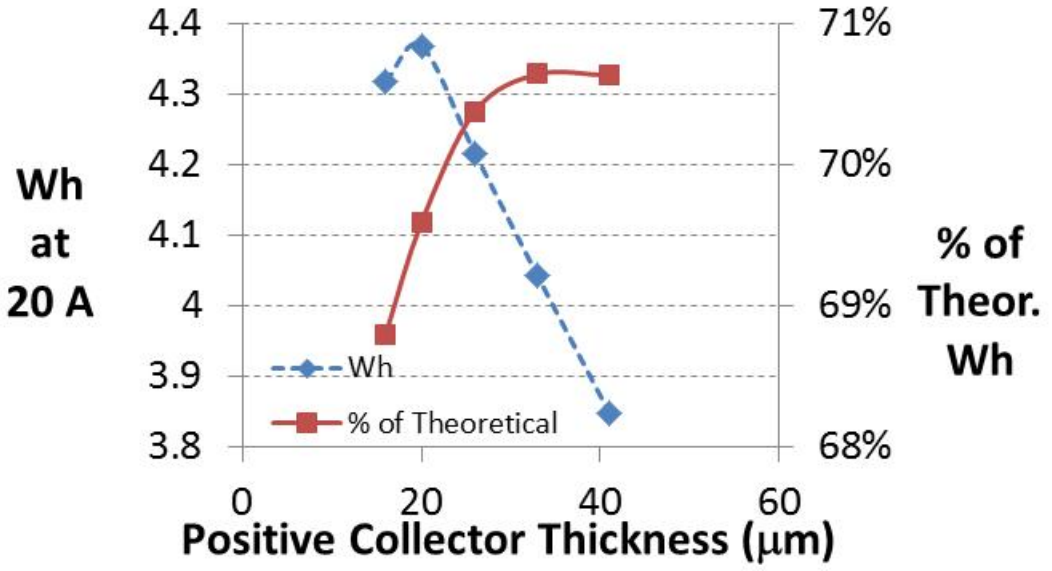

Figure 9. Effect of positive current collector thickness on available energy for a 20 A discharge.

High Power Cell with Varying Tab Position. In this cell design the tab of the negative electrodes is positioned at the outer radius of the jellyroll and the effect of the positive tab

position is studied. The positive electrode design is shown in Figure 10. A 20 micron thick positive collector and 12 micron negative collector were used.

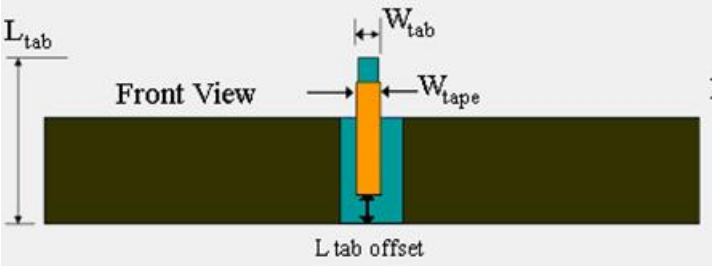

Figure 10. Electrode design for adjustable tab position.

For a 20 A discharge there was only about 10% variation in available energy (see Figure 11). The cell temperatures at end of discharge ranged from 55 to 59 °C with the low value corresponding to the positive tab position halfway from the core at the high value when the tab is at the ends. The optimal tab position is at the middle of the positive (see Figure 10). The effect of tab position becomes more pronounced at higher discharge currents especially if the simulation is stopped when the cell reaches 60 °C. For a 26 A discharge, there is greater than 40% variation in available energy (see Figure 12) with a pronounced optimum for the tab at the middle of the positive.

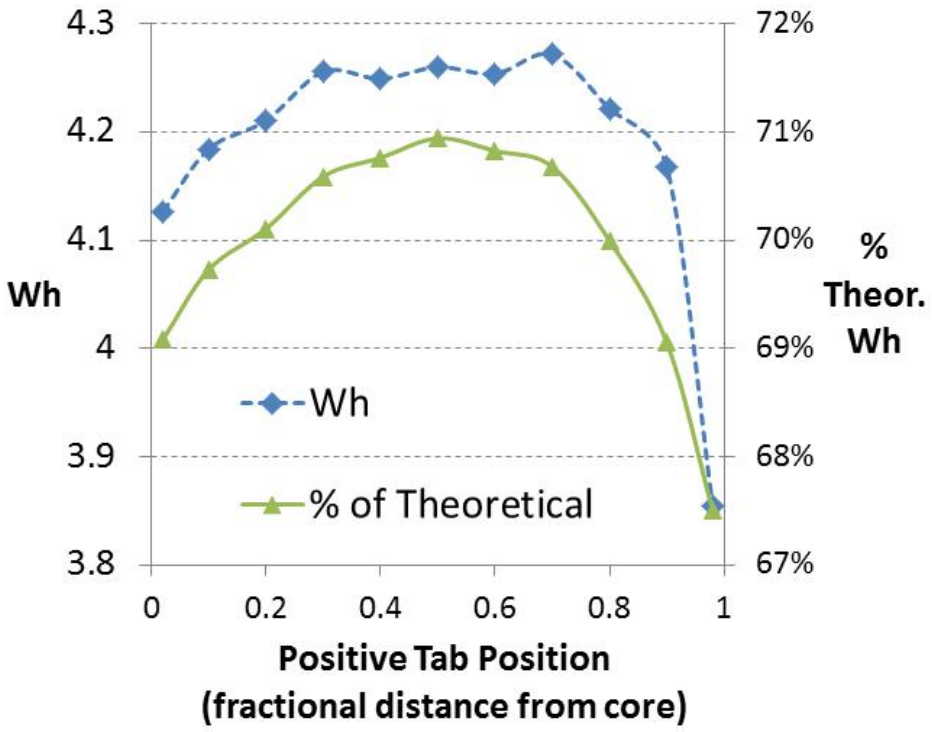

Figure 11. Effect of positive tab position on available energy and % of theoretical energy for 20 A discharge.

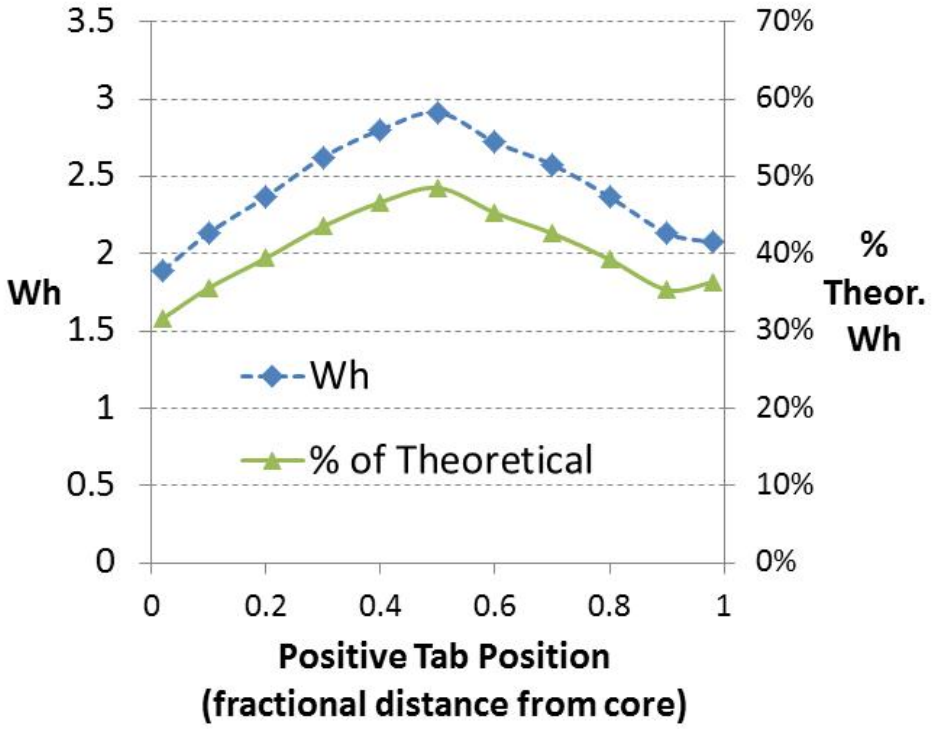

Figure 12. Effect of positive tab position on available energy and % of theoretical energy for 26A discharge with 60 °C limit.

High Power Cell with Multiple Tabs. In this cell design an electrode configuration with edge tabs is used (see Figure 13). Increasing the number of positive tabs to two with one negative tab provides a significant benefit (see Figure 14) while further increases in number of tabs provides only a marginal benefit in capacity and voltage.

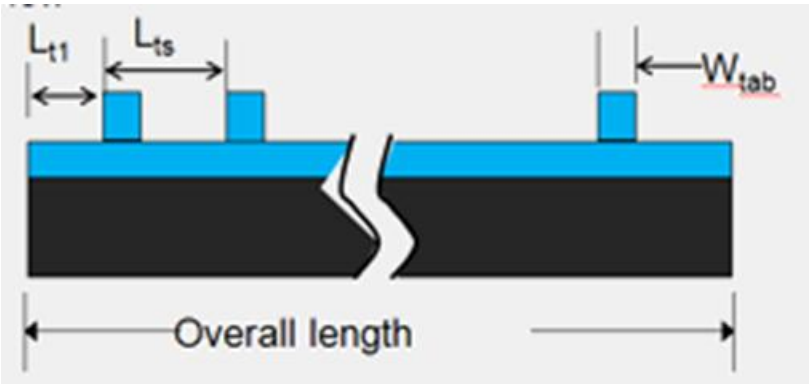

Figure 13. Electrode design with multiple edge tabs.

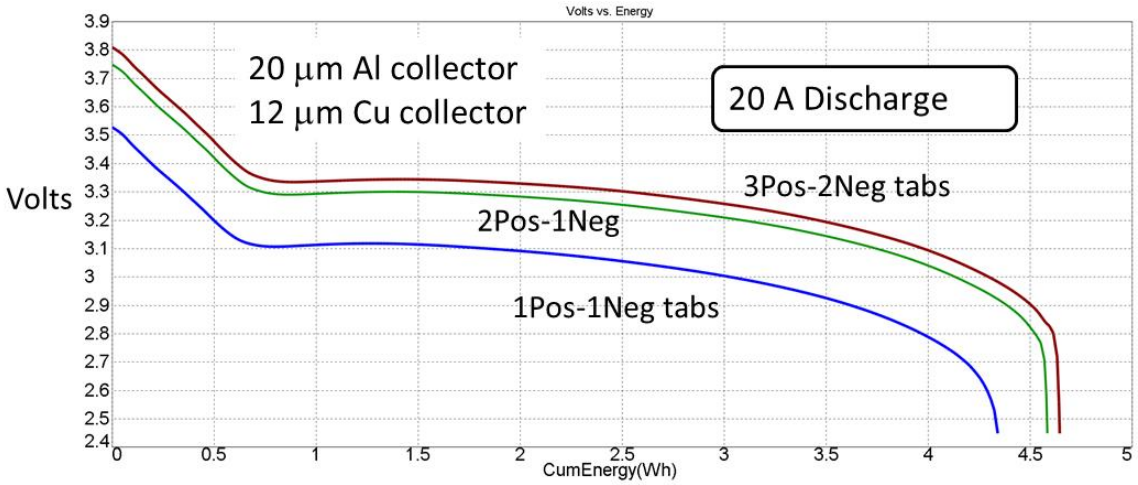

Figure 14. Effect of number of edge tabs on available capacity.

Conclusions

For 18650-size, high-energy cells with maximum discharge rates around 2 C, the current collector does not introduce large voltage losses. Thin collectors are suitable and tab design is not critical.

For 18650-size, high-power cells with current collectors having same resistance there is an optimal collector thickness to maximize available energy. If an end tab electrode design is used then the tabs at opposite ends is preferable over tabs at same ends. If the negative tab is at one end and the positive tab position can move, then the optimal position is midway along the length of the positive.

If multiple tabs can be used, then the ohmic drop in the collectors can be made very small with just a few tabs.

Acknowledgments

This work was funded in part by US Department of Energy – Office of Vehicle Technologies, program managers David Howell and Brian Cunningham, as part of the Computer-Aided Engineering of Batteries (CAEBAT) program under subcontract ZCI-1-40497-01 with the National Renewable Energy Laboratory under the supervision of Dr. Kandler Smith.

References

1. J. Reimers *J. Power Sources*, **158**, 663 (2006).
2. U. Kim, C. Shin, and C.-S. Kim, *J. Power Sources*, **189**, 841 (2009).
3. M. Doyle, T. F. Fuller, and J. Newman, *J. Electrochem. Soc.*, **140**, 1526 (1993).
4. T. F. Fuller, M. Doyle, and J. Newman, *J. Electrochem. Soc.*, **141**, 1 (1994).