Modeling a Commercial Li-Ion Cell with Basic Cell Design Inputs Available from Supplier

Introduction

A large number of companies (such as system integrators and/or auto OEMs) procure Li-ion cells from suppliers and therefore detailed information about Li-ion cell design, for instance electrode thickness, porosity, weight fraction etc., or material properties are not easily available to engineers of these companies. In such a situation, how can engineers rely on physics-based models that require this information to capture cell behavior? In this example, we are “enacting” as engineers who can get some basic information about cell design from their suppliers. We are then showcasing how can such engineers effectively utilize AutoLion™ to capture characteristics of their specific cells.

Problem Definition

EC Power bought 18650 cells from a commercial Li-ion cell manufacturer (one of the three largest manufacturers in the world). From manufacturer’s spec sheet, it was found that cell has NMC/C based chemistry. EC Power then cut open a cell to measure basic cell design specifications that should be easily available or can be extracted from the information engineers can get from cell suppliers. Table 1 summarizes the design parameters we have measured in our lab. For other cells, performance is measured as a function of temperature using a pulse protocol. AutoLion is then used with measured design parameters as inputs along with in-built material database of AutoLion for NMC and Graphite to simulate the performance.

Technology Used

AutoLion-1D™

Setup

- A 2.2 Ah NMC/graphite 18650 cell designed using measured design inputs.
- In-built material database in AutoLion for NMC and Graphite is used. Material properties such as exchange current density, Li diffusion coeff in solid particles, OCVs etc. are incorporated as a function of temperature and Li stoichiometry in the database.
- Electrode tortuosity, SEI resistance and contact resistance are the only parameters tweaked as their measurements are not available for the specific cell in question. These parameters once chosen remain untouched for various temperatures and pulse profiles at various temperatures.
- Dynamic performance simulation carried out using current input profile shown in Figure 1. Simulations carried out at 25°C and 0°C.

Table 1. Design inputs measured (or assumed) for a commercial 18650 cell

<table>
<thead>
<tr>
<th>Property</th>
<th>Negative Electrode</th>
<th>Separator</th>
<th>Positive Electrode</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thickness (um)</td>
<td>80</td>
<td>20*</td>
<td>78</td>
</tr>
<tr>
<td>Porosity+</td>
<td>26%</td>
<td>39%*</td>
<td>28%</td>
</tr>
</tbody>
</table>

+ Taken from Celgard standard spec sheet assuming a Celgard 2320 separator is used
+ Can be calculated if weight of active material, binder and filler is available (typically can be obtained from a supplier). In this case study, measurements are done using standard porosimetry method

Results

Figure 1: Input current profile used for the experiment.
Figure 2: Simulated and measured voltage response to the input current profile for cell with 60% starting SOC at 25°C. Experimental data is average of two cells.

Figure 3: Simulated and measured voltage response to the input current profile for cell with 40% starting SOC at 25°C. Experimental data is average of two cells.

Figure 4: Simulated and measured voltage response to the input current profile for cell with 60% starting SOC at 0°C. Experimental data is average of two cells.

Figure 5: Simulated and measured voltage response to the input current profile for cell with 60% starting SOC at 0°C. Experimental data is average of two cells.

User Benefits

- AutoLion™ can be easily used by users to reliably model a commercial cell for which they may not have detailed design or material-level information available. Thereby, AutoLion™ offers users the ease-of-use of empirical models but in addition the flexibility and accuracy of physics-based models.
- AutoLion™ can capture performance of Li-ion cells with a wide range of chemistries with less than 5% of error compared to the experimental data. Further reduction in error is easily possible, though not attempted in this case study.
- Changing parameters in AutoLion to obtain a good match with data is very easy and effective.
- EC Power, in addition to its AutoLion™ software suite, offers a comprehensive material property measurement services. Not only key material properties can be measured as a function of SOC and temperature but also can be incorporated in customer-specific version of AutoLion™.