AutoLion

a Suite of Thermally Coupled Battery Simulation Tools
for large-format Li-ion Batteries

Model Comparison with Experiments

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AutoLion™: Unprecedented Accuracy in Capturing Li-ion Battery Performance

- Cell: 2.2 Ah 18650 cell with NMC/graphite chemistry
- AutoLion™ captures battery performance and temperature profile with great accuracy

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Dynamic Pulse Profile Experiments

- Cell: 1.2 Ah high power 18650 cell
- Chemistry: NMC/Graphite
- Experiments carried out at 25°C and 0°C inside an environmental chamber
- 2 cells repeat

Cell Design Specs

<table>
<thead>
<tr>
<th></th>
<th>Negative electrode</th>
<th>Separator</th>
<th>Positive electrode</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thickness (um)</td>
<td>40</td>
<td>25</td>
<td>35</td>
</tr>
<tr>
<td>Porosity</td>
<td>56%*</td>
<td>40%</td>
<td>50%*</td>
</tr>
<tr>
<td>Active material wt fraction (%)</td>
<td>94%</td>
<td>NA</td>
<td>94%</td>
</tr>
<tr>
<td>Electrolyte:</td>
<td>1.2M LiPF6 in EC/DMC</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Calculated value

Input Current Profile

1 sec charge-discharge pulse at 1C, 2C, 5C and 10C followed by 10 sec pulses at the same C-rates
**AutoLion™ Model Results at 25°C**

**Environmental chamber temperature: 25°C**

Cell Starting SOC = 90%

Cell Starting SOC = 60%

- Very repeatable data; no significant difference in the 2 cell response.
- In-built material database as a function of T and concentration is used for simulations. The only parameters tuned are electrode tortuosity, contact resistance and SEI resistance.
- Simulation results matches very well with data with **maximum error being less than 2% error**; showcasing excellent accuracy of AutoLion™ under Dynamic Conditions.

*SOC is defined as capacity left to discharge/design capacity (C/20) at 25°C*
AutoLion™ Model Results at 0°C

Environmental chamber temperature: 0°C

Cell Starting SOC = 90%

Cell Starting SOC = 60%

In-built material database as a function of T and concentration is used for simulations. All the physical parameters (such as contact resistance or electrode design parameter) remain untouched and are the same as for 25°C dynamic simulations.

Simulation results matches very well with data with maximum error being less than 5% error at 0°C; showcasing excellent accuracy of AutoLion™ under dynamic conditions.

SOC is defined as capacity left to discharge/design capacity (C/20) at 25°C
Experiment with 2.2 Ah 18650 Panasonic Cell

- Cell: 2.2 Ah energy dense (PHEV-type) 18650 cell from Panasonic
- Chemistry: NMC/Graphite
- Experiments carried out at 25°C and 0°C inside an environmental chamber

Cell simulation in AutoLion

- EC Power has characterized various cells in 18650 formats with high power (~1.2 Ah), PHEV (~2.2 Ah) and high energy (~2.8 Ah) and have developed a “representative” cell design file for these cells (available to AutoLion users)
- For simulation of Panasonic cell, we have used our generic cell design file for PHEV cell (design parameters as following)

<table>
<thead>
<tr>
<th></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>40%</td>
<td>28%</td>
</tr>
<tr>
<td>Electrode loading (mAh/cm²)</td>
<td>4.5</td>
<td>NA</td>
<td>3.9</td>
</tr>
<tr>
<td>Electrolyte:</td>
<td>1.2M LiPF6 in EC/DMC</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- 10 sec charge-discharge pulse at 1C, 2C, 5C and 10C
AutoLion™ is capable of capturing dynamic response of commercial cells even when detailed information of cell design is not available. Easy to work with and robust software.

The only parameters tuned are electrode tortuosity, contact resistance and SEI resistance. Rest material properties are from material database. Between this case (2.2 Ah cell) and the 1.2 Ah cell simulation (slides 2-4), only contact resistance is different; rest of the material properties are exactly the same.

Simulation results matches very well with data with maximum error being less than 2% error; showcasing excellent accuracy of AutoLion™ under dynamic conditions.
In-built material database as a function of T and concentration is used for simulations. All the physical parameters (such as contact resistance or electrode design parameter) remain untouched and are the same as for 25°C dynamic simulations.

- Simulation results matches very well with data with maximum error of ~5% error at 0°C; showcasing excellent accuracy of AutoLion™ under dynamic conditions.

\[ SOC \text{ is defined as capacity left to discharge/design capacity (C/20) at } 25^\circ C \]
AutoLion™ Life Model Validation

- **A123 ANR26650M1-B**: Graphite-LFP high power cell
- Capacity 2.3~2.5Ah

<table>
<thead>
<tr>
<th>Thickness (µm)</th>
<th>Anode</th>
<th>Separator</th>
<th>Cathode</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity</td>
<td>0.41</td>
<td>0.40</td>
<td>0.63</td>
</tr>
<tr>
<td>Particle radius (µm)</td>
<td>5</td>
<td>/</td>
<td>36.5[1]</td>
</tr>
</tbody>
</table>

25°C

1C CC cycling at 25°C
(symbols are experimental data)

C/10 discharge test at
Month
0
1
3
6
9
12 (4598 cyc)

Life predictions against third party data* for LFP/C 26650 cell


*J. Wang et al., J Power Sources, 196, 3942 (2011)
AutoLion™ Life Model Validation

AutoLion™ can not only capture cell behavior but also the voltage decay of each electrode with cycling over a wide range of operating conditions.

Cell chemistry: NMC/graphite

Cathode voltage plots

Anode voltage plots

25°C 1C characterization

25°C 1C characterization

25°C 1C characterization

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For more information on EC Power and its products, contact us at:

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