New Techniques for Thermo-electrochemical Analysis of Lithium-ion Batteries for Space Applications

W. Walker and H. Ardebili

Presented By
William Walker (NASA/JSC)

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• Introduction to the Topic
• Lithium-ion Battery (LIB) Charge/Discharge Heat Transfer Mechanisms
• Thermal Desktop Model Development
• Results:
  – Case 1, final
  – *Case 2 not presented
  – *Case 3 presenting, still pending final review
• Conclusion and Future Work
• References
• Disclaimer Statements
  – This work was inspired by, but is not affiliated with the NASA/Boeing ISS LIB replacement battery project
  – All results are part of on-going research conducted for academic purposes with my graduate advisor (H. Ardebili, co-author)
Section 1:
Introduction to the Topic
Introduction to the Topic

• The need for renewable energy, more efficient energy consumption, and the incorporation of advanced energy storage technologies escalates each year with the increasing consumption of non-renewable resources and decreasing availability of said resources.
• The need to survive in space environments where fuel sources are not readily available also leads to a high dependence on advanced energy storage capabilities.
• Advanced energy storage devices are compared on a Ragone plot.
• LIBs are increasing in popularity and were chosen as replacement batteries for some of the ISS Ni-H$_2$ batteries because of their superior performance in:
  – Energy density and power density
  – Ionic conductivity
  – Operating and storage temperature ranges
  – Life cycles and shelf life

• The selection of LIBs for use in satellites and now the ISS exemplifies the need to predict thermal performance in orbital environments; for batteries, thermal performance is a function of environment and local heating rates

• Note that the thermal analysis of LIBs is not new:
  – Sophisticated numerical methods began in 1985
  – Presently it is well known that the optimal way to perform this type of analysis is through a coupled (or multi-physics) methodology which combines the effects of:
    • Heating through electrochemical reactions
    • Heating through environmental factors
  – This type of analysis is easily conducted for simple thermal environments in multi-physics software like COMSOL; however,
    • Implementing orbital environments requires more specialized software (Thermal Desktop)
    • The problem is that TD is not readily set up to incorporate the complexities of local heating from thermo-electrochemical reactions

• Research seeks to develop a coupled thermo-electrochemical model in thermal orbital analysis software of a Lithium-ion battery whose local heat generation rate is a function of the environment (orbital or sink based), local temperature, and depth of discharge
  – Rather than a power profile that is provided prior to analysis
  – Essentially, the power profile should be a function of the model itself
Section 2:
LIB Charge/Discharge Heat Transfer Mechanisms
LIB Basics:
- LIBs store and provide energy through a series of charge/discharge processes that occur through the simultaneous electrochemical reactions between the electrodes and the flow of electrons through a completed circuit
- Typical LIB components: Anode, Cathode, Electrolytic Material, Separator, and Current Collectors

As with any object, the three modes of heat transfer apply: convection, conduction, radiation

In 1985 Bernardi et. al. developed a basic equation to represent the local heat generated in the cells of a LIB as a result of electrochemical processes (captures heat due to Ohmic losses, charge-transfer at the interface, and mass transfer limitations):

\[
Q = I \left( E_{OC} - E - T \frac{\partial E_{OC}}{\partial T} \right) \tag{1}
\]

- \( I \) is the total current
- \( E_{OC} \) is the open circuit potential
- \( E \) is the working voltage
- \( T \) is the local temperature
Section 3:
Thermal Desktop Model Development
Thermal Desktop Model Development

• Before conducting an orbital analysis, development of a simple non-orbital (sink temperature based) TD model of a LIB with Bernardi’s equation for local heating was needed.

• Chose a convection/radiation numerically based assessment of a 185 Ah LIB conducted by Chen et. al. (primary source) who also utilized Bernardi’s equation for local heating.

• In short, recreated a previously conducted numerical analysis in TD to determine if TD had the ability to be coupled with thermo-electrochemical math models (i.e. Bernardi’s equation).
Thermal Definition:
- Geometries and material properties provided in table
- Convection represented through a 300 K boundary node connected to the exterior encasement surfaces with a natural convection conductor (4.3-10 W/m²K depending on location and DoD)
- External surfaces set to radiate to a 300 K sink temperature
- Assumed 200 W/m²K contact between the core, the electrolytic layer, and the encasement

<table>
<thead>
<tr>
<th>Variable</th>
<th>Density (kg/m³)</th>
<th>Heat Capacity (J/kg/K)</th>
<th>Thermal Conductivity (W/m/K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminum (Encasement)</td>
<td>2770</td>
<td>875</td>
<td>170</td>
</tr>
<tr>
<td>Liquid Electrolyte (Contact Layer)</td>
<td>1130</td>
<td>2055</td>
<td>0.60</td>
</tr>
<tr>
<td>Core Region (Cells)</td>
<td>3264</td>
<td>1194</td>
<td>1.04, 24.8, 24.8</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variable</th>
<th>Magnitude</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Size of Core Region</td>
<td>19.08 x 10.00 x 10.00</td>
<td>cm³ cm³ cm³</td>
</tr>
<tr>
<td>Thickness of Encasement</td>
<td>0.07</td>
<td>cm</td>
</tr>
<tr>
<td>Thickness of the Contact Layer</td>
<td>0.05</td>
<td>cm</td>
</tr>
<tr>
<td>Ambient Temperature</td>
<td>300</td>
<td>K</td>
</tr>
<tr>
<td>Theoretical Capacity</td>
<td>185</td>
<td>Ah</td>
</tr>
<tr>
<td>Change in EOC vs. Time</td>
<td>0.00022</td>
<td>V/K</td>
</tr>
<tr>
<td>Encasement Emissivity</td>
<td>0.25</td>
<td>N/A</td>
</tr>
</tbody>
</table>
• Local heating applied to the 125 “core” region nodes (load divided volumetrically)
• Applying Bernardi’s equation:
  – Current was based on a 185 Ah battery and which discharge case was under consideration
    • 1C = 60 Minutes Discharge Time @ I = 185 A
    • 2C = 30 Minutes Discharge Time @ I = 370 A
    • 3C = 20 Minutes Discharge Time @ I = 555 A
  – Open Circuit Potential and Working Voltages for 1, 2, and 3 C discharge profiles provided in the image below
  – Developed arrays of the voltage vs. DoD location for each discharge case
  – Developed TD logic to update the local heating on the “core” region after every iteration in the solution process
  – *Case 3 implemented logic to update the local T value of Bernardi’s equation after each iteration

\[ Q = I \left( E_{OC} - E - T \frac{\partial E_{OC}}{\partial T} \right) \]  (1)
Thermal Desktop Model Development

Test Case Matrix

<table>
<thead>
<tr>
<th>Case ID</th>
<th>Case Type</th>
<th>Discharge Rate (C)</th>
<th>Total Discharge Time (s)</th>
<th>Current (A)</th>
<th>Convection (W m⁻² K⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1-3C-NAT</td>
<td>Case 1</td>
<td>3</td>
<td>1200</td>
<td>555</td>
<td>Natural</td>
</tr>
<tr>
<td>C1-2C-NAT</td>
<td>Case 1</td>
<td>2</td>
<td>1800</td>
<td>370</td>
<td>Natural</td>
</tr>
<tr>
<td>C1-1C-NAT</td>
<td>Case 1</td>
<td>1</td>
<td>3600</td>
<td>185</td>
<td>Natural</td>
</tr>
<tr>
<td>C1-3C-20</td>
<td>Case 1</td>
<td>3</td>
<td>1200</td>
<td>555</td>
<td>20 (Forced)</td>
</tr>
<tr>
<td>C1-3C-50</td>
<td>Case 1</td>
<td>3</td>
<td>1200</td>
<td>555</td>
<td>50 ( Forced)</td>
</tr>
<tr>
<td>C1-3C-100</td>
<td>Case 1</td>
<td>3</td>
<td>1200</td>
<td>555</td>
<td>100 (Forced)</td>
</tr>
<tr>
<td>C1-3C-200</td>
<td>Case 1</td>
<td>3</td>
<td>1200</td>
<td>555</td>
<td>200 (Forced)</td>
</tr>
<tr>
<td>C1-3C-300</td>
<td>Case 1</td>
<td>3</td>
<td>1200</td>
<td>555</td>
<td>300 (Forced)</td>
</tr>
<tr>
<td>C2-3C-NAT</td>
<td>Case 2</td>
<td>3</td>
<td>1200</td>
<td>555</td>
<td>Natural</td>
</tr>
<tr>
<td>C2-2C-NAT</td>
<td>Case 2</td>
<td>2</td>
<td>1800</td>
<td>370</td>
<td>Natural</td>
</tr>
<tr>
<td>C2-1C-NAT</td>
<td>Case 2</td>
<td>1</td>
<td>3600</td>
<td>185</td>
<td>Natural</td>
</tr>
<tr>
<td>C3-3C-NAT</td>
<td>Case 3</td>
<td>3</td>
<td>1200</td>
<td>555</td>
<td>Natural</td>
</tr>
<tr>
<td>C3-2C-NAT</td>
<td>Case 3</td>
<td>2</td>
<td>1800</td>
<td>370</td>
<td>Natural</td>
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<tr>
<td>C3-1C-NAT</td>
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<tr>
<td>C3-3C-20</td>
<td>Case 3</td>
<td>3</td>
<td>1200</td>
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<tr>
<td>C3-3C-300</td>
<td>Case 3</td>
<td>3</td>
<td>1200</td>
<td>555</td>
<td>300 (Forced)</td>
</tr>
</tbody>
</table>

• **Case 1: Exact Replication of Chen’s Study**
  – EOC and E update in the Q equation (Bernardi’s) after each iteration. I, T, and \( \frac{\partial E_{oc}}{\partial T} \) held constant

• **Case 2: No-Logic, Constant/Averaged Local Heating Applied**
  – Constant local heating applied based on average of entire DoD

• **Case 3: Attempted Improvement to Chen’s Numerical Thermal Model**
  – EOC, E, and T update in Q equation (Bernardi’s) after each iteration. Updated thermophysical properties to include an electrolytic layer between the electrodes
Section 4: Thermal Desktop Results
Case 1 Natural Convection Results

TD Case 1 Results Compared to Chen's Results: Natural Convection

TD = Thermal Desktop Results
Chen = Chen’s Results

Temperature (K)

Depth of Discharge (DoD)
Case 1 Forced Convection Results

TD Case 1 Results Compared to Chen's Results: Forced Convection

TD = Thermal Desktop Results
Chen = Chen’s Results
Conv = Convection (W/m²/K)

Temperature (K)

Depth of Discharge (DoD)
Case 3 Natural Convection Results

*Case 3 results pending final review*
Case 3 Forced Convection Results

*Case 3 results pending final review*
Section 5:
Conclusion and Future Work
Conclusion and Future Work

- The overall goal of this study was achieved:
  - Replicated the numerical assessment performed by Chen et. al. (2005)
  - Displayed the ability of Thermal Desktop to be coupled with thermo-electrochemical analysis techniques such that the local heat generated on the cells is a function of the model itself using logic blocks and arrays

- Differences in the TD temperature vs. depth of discharge profiles and Chen’s was most likely due to differences in two primary areas:
  - Contact regions and conductance values
  - Differences in density and specific heat values

- The model results are highly dependent on the accuracy of the material properties with respect to the multiple layers of an individual cell

- Future work:
  - Develop and contact a highly controlled test where all factors are known – replicate test in Thermal desktop – compare to provide final validation of these new techniques
  - Implement these techniques into an orbital scenario/model (ultimate goal) to investigate the effects of this analysis technique combined with orbital analysis techniques
  - Develop more detailed model to provide better definition of where the hot spots will occur (similar to work being done in COMSOL)
  - Could we then?
    - Predict beta angles and solar conditions which could invoke a thermal run-away condition
    - Make more accurate performance predictions to minimize necessary thermal control/protection
    - Implement thermal considerations into the design of the battery rather than waiting until the battery is complete and then adding passive/active thermal cooling/heating
Section 6:
References
References