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

W. Walker and H. Ardebili

Presented By
William Walker (NASA/JSC)

Thermal & Fluids Analysis Workshop
TFAWS 2013
July 29-August 2, 2013
Kennedy Space Center
KSC, FL
Presentation Overview

- 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.

Image retrieved belongs to the US Defense Logistics Agency.
LIBs are increasing in popularity and were chosen as replacement batteries for some of the ISS Ni-H₂ 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 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):

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

- \(I\) is the total current
- \(E_{OC}\) is the open circuit potential
- \(E\) is the working voltage
- \(T\) is the local temperature

Images retrieved from electronics.howstuffworks.com
Section 3:
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 Desktop Model Development

• 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>cm<em>cm</em>cm</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>
Thermal Desktop Model Development

- 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

\[ Q = I \left( E_{OC} - E - T \frac{\partial E_{OC}}{\partial T} \right) \quad (1) \]
### 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>
</tr>
<tr>
<td>C3-1C-NAT</td>
<td>Case 3</td>
<td>1</td>
<td>3600</td>
<td>185</td>
<td>Natural</td>
</tr>
<tr>
<td>C3-3C-20</td>
<td>Case 3</td>
<td>3</td>
<td>1200</td>
<td>555</td>
<td>20 (Forced)</td>
</tr>
<tr>
<td>C3-3C-50</td>
<td>Case 3</td>
<td>3</td>
<td>1200</td>
<td>555</td>
<td>50 (Forced)</td>
</tr>
<tr>
<td>C3-3C-100</td>
<td>Case 3</td>
<td>3</td>
<td>1200</td>
<td>555</td>
<td>100 (Forced)</td>
</tr>
<tr>
<td>C3-3C-200</td>
<td>Case 3</td>
<td>3</td>
<td>1200</td>
<td>555</td>
<td>200 (Forced)</td>
</tr>
<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