Predicting Temperatures in a Li-ion Battery using a Model-based Prognostics

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Funded By
NASA Aeronautics Research Mission Directorate (ARMD) Convergent Aeronautics Solutions (CAS) Project, SPARRCI sub-project.

Presentation date: 11/18/2020
Outline

1. Project Overview
2. Li-ion Failure Introduction
3. Li-ion Failure Modeling and Simulation
4. Prognostics Overview
5. Li-ion Discharge Time and Temperature Estimation
6. Conclusion
Today’s Bulky Pack Designs

Pack penalty: 23%  Additional mass for “safe” packs  Safe pack penalty: 61%

Safety Testing - Thermal Runaway
Problem Formulation

Emerging Electric Aircraft need Better and Safer Batteries

- Current Monitored Battery Parameters
  - Voltage
  - Current
  - Temperature

- Consequence of Unmitigated Cell Thermal Runaway Events
  - Fire
  - Explosion
  - Debris

✓ Internal Monitoring
✓ Failure prevention via internal fault detection & mitigation
Project Overview

Different components

1. Experimental
   - Embedded Sensors

2. Modeling
   - Detect and Model Fault precursors
   - Develop state estimation and prognostic algorithms
   - Battery Management System (BMS) Capable of Fault Mitigation
Li-ion (an Overview)

- **Li-ion Chemistry**
  - Cathode (LCO/NMC/LFP)
  - Anode (Graphite/Lithium)
  - Electrolyte ($\text{LiCF}_3\text{SO}_3$, $\text{LiPF}_6$ in EC/DMC)
  - Separator (PP/Al$_2$O$_3$)

  **Anode reaction**
  \[ \text{Li}_x\text{C} \rightarrow \text{C} + x\text{Li}^+ + xe^- \]

  **Cathode reaction**
  \[ \text{Li}_{1-x}\text{CoO}_2 + x\text{Li}^+ + xe^- \rightarrow \text{LiCoO}_2 \]
Common Sources of Thermal Runaway

- Mechanical abuse
  - Deformation
  - Crash
- Electric abuse
  - Overdischarge
  - Overcharge
  - Dendrite growth
  - Internal short circuit
- Thermal abuse
  - Overheating
  - High Temperature
- Thermal runaway

A Cell’s Path to Thermal Runaway

<table>
<thead>
<tr>
<th>Process</th>
<th>Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>SEI decomposition</td>
<td>69°C</td>
</tr>
<tr>
<td>Anode/electrolyte reaction</td>
<td>100°C</td>
</tr>
<tr>
<td>separator melt</td>
<td>130°C</td>
</tr>
<tr>
<td>electrolyte decomposition</td>
<td>200°C</td>
</tr>
<tr>
<td>Electrolyte/cathode reaction</td>
<td>300°C</td>
</tr>
</tbody>
</table>

Thermal runaway

Finite Element Failure Modeling

**Inputs**
- Materials
- Chemistry
- Geometry
- Cell Configuration
- Experimental Condition

**Phenomena**
- Thermal
- Lithium Plating
- Capacity Fade
- Dendrite Growth
- Chemical Decomposition
- Overcharge
- Shrinking Core Model

**Outputs**
- Cell Temperature
- Cell Potential
- Cell Capacity
- Discharge Time
- Cycle
A typical model for Li-ion

Electrolyte Transport

\[ \frac{\partial \varepsilon_c c_e}{\partial t} - \nabla \cdot (D_{\text{rev}}^{\text{eff}} \nabla c_e) - \frac{1 - t_0}{F} a_s j_n = 0 \]

Electrolyte Potential

\[ \nabla \cdot \left( \kappa_e^{\text{eff}} \nabla \phi_e - \frac{2RT \kappa_e^{\text{eff}}}{F} (1 - t_0^0) \left( 1 + \frac{d \ln f_\pm}{d \ln c_e} \right) \nabla \ln c_e \right) + a_s j_n = 0 \]

Electrode Potential

\[ \nabla \cdot (\sigma_s \nabla \phi_s) - a_s j_n = 0 \]

Reaction Kinetics

\[ j_n = i_0 \left( \exp \left( \frac{\alpha_a F}{RT} (\phi_s - \phi_e - U_{\text{eq}}) \right) - \exp \left( - \frac{\alpha_c F}{RT} (\phi_s - \phi_e - U_{\text{eq}}) \right) \right) \]

\[ i_0 = k c_e^{\alpha_a} (c_{\text{max}} - c_{r=R_s})^{\alpha_a} c_e^{\alpha_c} |_{r=R_s} \]

Particle Diffusion

(Shrinking Core Model)

\[ \frac{\partial c_\alpha}{\partial t} = \frac{1}{r^2} \left( D_\alpha r^2 \frac{\partial c_\alpha}{\partial r} \right) \]

Degradation Model

\[ i_{\text{loc, SEI}} = -(1 + HK) \frac{J j_{\text{loc, 1C, ref}}}{\exp \left( \frac{\alpha_{\text{SEI}} F}{RT} \right) + \frac{q_{\text{SEI}} F}{i_{\text{loc, 1C, ref}}}} \]

Thermal Model

\[ \rho C_p \frac{\partial T}{\partial t} = q_{\text{rev}} + q_{\text{irr}} + q_{\text{ohm}} + q_{\text{chem}} - q_{\text{radiation}} - q_{\text{convection}} \]
Finite Element Model Simulations

SEI formation and the loss of useable lithium

- Loss of Lithium
- Increased Impedance
- Change in Exothermic Profile

SEI not only affects Capacity but also the Internal Cell Temperature
Lithium Dendrite Growth on a Lithium Metal Anode

Internal Short Circuit by Lithium Dendrites can cause Thermal Runaway

Monroe, C., & Newman J. Journal of The Electrochemical Society 150, no. 10 (October 1, 2003): A1377–84. DOI: 10.1149/1.1606686
Dendrite Growth in a Graphite anode

Lithium plating coupled with lithium dendrite growth represents internal short circuit

Abused Graphite Anodes could lead to Thermal Runaway
• Chemical decomposition reactions are exothermic
• Peak heating rates are activated at different temperatures
• Temperature rise during short circuit is often followed by a chemical thermal runaway

Battery Materials are Exothermic and Sensitive to the Internal Cell Temperature
Effect of Chemical Decomposition on the Internal Temperature on a Nominal Li-ion Cell
Estimating Temperature for Predicting Failure

- Finite Element simulations is used to identify important precursors
- Temperature is easy and cheaper to monitor
- A BMS with internal temperature monitoring and a physics-based estimation algorithm could be used for failure prediction

\[
\frac{\partial T}{\partial t} = \frac{1}{\rho C_p} \left[ q_{\text{rev}} + q_{\text{irr}} + q_{\text{ohm}} + q_{\text{chem}} \right]
\]

- Electrochemical
- Thermodynamic
- Ohmic and short-circuit
- Chemical decomposition
Battery Prognostics
Model Based Architecture

1. System receives inputs, produces outputs
2. Identify active damage mechanisms
3. Estimate current state and parameter values
4. Predict EOL and RUL as probability distributions

System receives inputs, produces outputs

Fault Detection Isolation & Identification

Estimation

Prediction

System

\[ y_k \]

\[ u_k \]

\[ p(x_k, \theta_k | y_{0:k}) \]

\[ p(EOL_k | y_{0:k}) \]

\[ p(RUL_k | y_{0:k}) \]
Battery Thermal Prognostics

Modifying the Model for Temperature

Two State Estimation Blocks can estimate Cell Voltage, Discharge Time, Cycle Life, and Temperature Thresholds
Current Goal for Prognostics

Evolution of the Material Properties

- Predict Temperature for Thermal Runaway
- Predict Internal Cell Temperature
- Predict thermal runaway

Current State

Time/cycle

Cycle
The estimation error reduces as the discharge time increases.
Data from a Short Test Flight

“Noisy” sensor data

Smoothed data used for prognostics

Data pre-processing is needed for accurate estimation
Preliminary Results for EOD Estimation

Applying Prognostics Algorithm on a Short Test Flight Profile

The Distribution of the End-of-Discharge Estimation shows that the Algorithm is working correctly.
Preliminary Results for Temperature Estimation

Applying Prognostics Algorithm on a Short Test Flight Profile

Temperature variation on a nominal and fresh cell is not significant
Summary

• Failure modes identification
• Finite Element Modeling of Failure modes
• Identification of temperature as a failure precursor
• Coupled a thermal model with battery prognostics algorithm
• Voltage and temperature estimation for a single cycle

Next Steps

• Estimating temperature over cycle life
• Estimating temperature for off-nominal behavior