Lithium-ion Batteries – towards Safety and Performance Interplay

Department of Mechanical Engineering

ENGR 491 – 506

AggiE Challenge Program

Fall semester, 2015
<table>
<thead>
<tr>
<th></th>
<th>Students</th>
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<tbody>
<tr>
<td>1</td>
<td>Alec Chandler Best</td>
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<td>2</td>
<td>Alexander Clay Ellis</td>
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<td>Andres Eduardo Crucetta Nieto</td>
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<td>Christopher Lewis Balhoff</td>
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<td>Colby Kenneth Sherman</td>
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<td>Jose Eduardo Mejia</td>
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Mentors

Faculty advisors:

- Dr. Partha P. Mukherjee (PI)
- Dr. Hong Liang

Graduate student mentors:

- Aashutosh Mistry
- Chien-Fan Chen
- Daniel Juarez-Robles
Lithium - Ion Batteries

Electrical energy is generated by conversion of chemical energy via redox reactions at the anode and cathode.

Schematic of Lithium ion battery

1. Source: www.alibaba.com
2. Source: HowStuffWorks
Electrode Preparation
Objective

Data-driven model for cell performance

Understanding of materials-transport-interface interactions in energy storage and conversion, particularly within electrochemical energy storage of Lithium Ion batteries.

Parameters selected for modeling Li-ion cell performance

<table>
<thead>
<tr>
<th>Input</th>
<th>Output</th>
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<tbody>
<tr>
<td>Active Material Composition</td>
<td>Voltage</td>
</tr>
<tr>
<td>Drying Temperature</td>
<td>Capacity</td>
</tr>
<tr>
<td>C-Rate</td>
<td></td>
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Scanning Electron Microscope (SEM) imaging was used for constructing a 3D STL.

STL rendering prior to 3D printing

3D printed demonstration
Coin Cell Fabrication

**Electrode Sheet Preparation**
- Aluminum foil cleaning
- Making the slurry
- Casting of the slurry
- Electrode drying

**Testing Coin Cells**
- CCCV charging protocol
  - (CCCV: constant current constant voltage)
- C-rate, Electrode mass

**Coin Cell Preparation**
- Cap, Case
- Li metal, Separator
- Gasket, Wave spring
- Electrolyte
Coin Cell Fabrication

- Slurry Mixing
- Coin Cell Assembly
- Electrode Casting

Coin Cell (type 2032)
**Cells Tested**

**Independent Variables:** Composition, Drying Temperature, C-Rate

<table>
<thead>
<tr>
<th>Case 1</th>
<th>Composition [AM %wt, CA %wt, Binder %wt]</th>
<th>Drying Temperature [°C]</th>
<th>C-Rate [1/hour]</th>
</tr>
</thead>
<tbody>
<tr>
<td>721</td>
<td>60</td>
<td>1C, C/2, C/5, C/20</td>
<td></td>
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<tr>
<td>Case 2</td>
<td>721</td>
<td>25, 60, 95</td>
<td>1C, C/2, C/5, C/20</td>
</tr>
<tr>
<td>Case 3</td>
<td>631, 721, 811</td>
<td>60</td>
<td>1C, C/2, C/5, C/20</td>
</tr>
</tbody>
</table>

**NMC**→ Nickel Manganese Cobalt

**Super C-65**→ Conductive Additive

**PVDF**→ Polyvinylidene Fluoride
Statistical Variation of Cells

- **C_Rate = 1C**
- **C_Rate = C/2**
- **C_Rate = C/5**
- **C_Rate = C/20**
Effect of Drying Temperature

C\_Rate = 1C

\begin{align*}
& T_{\text{drying}} = 25 ^\circ \text{C} \\
& 60 ^\circ \text{C} \\
& 95 ^\circ \text{C}
\end{align*}

C\_Rate = C/2

\begin{align*}
& T_{\text{drying}} = 25 ^\circ \text{C} \\
& 60 ^\circ \text{C} \\
& 95 ^\circ \text{C}
\end{align*}

C\_Rate = C/5

\begin{align*}
& T_{\text{drying}} = 25 ^\circ \text{C} \\
& 60 ^\circ \text{C} \\
& 95 ^\circ \text{C}
\end{align*}

C\_Rate = C/20

\begin{align*}
& T_{\text{drying}} = 25 ^\circ \text{C} \\
& 60 ^\circ \text{C} \\
& 95 ^\circ \text{C}
\end{align*}
Effect of Composition

- **C_Rate = 1C**
  - AM : CA : B
  - 80 : 10 : 10
  - 70 : 20 : 10
  - 60 : 30 : 10

- **C_Rate = C/2**
  - AM : CA : B
  - 80 : 10 : 10
  - 70 : 20 : 10
  - 60 : 30 : 10

- **C_Rate = C/5**
  - AM : CA : B
  - 80 : 10 : 10
  - 70 : 20 : 10
  - 60 : 30 : 10

- **C_Rate = C/20**
  - AM : CA : B
  - 80 : 10 : 10
  - 70 : 20 : 10
  - 60 : 30 : 10
Use of the Neural Networks:

1. Input of the data
2. Training of the NN
3. Testing data through Function Approximation and Regression Analysis

A neural network can use this experimental data to predict cell performance with different values for the same independent variables.
NN Training

```
1 // Input parameters
2 int LData=61;
3 Matrix trainSetInput;
4 Matrix trainSetInput.Load();
5 int Ls=5;
6 int Lo=2;
7 // Output parameters
8 Matrix trainSetTarget;
9 Matrix trainSetTarget.Load();
10 int Lo=2;
11 // Neural Network Creation
12 LayerNet net;
13 net.Create(Ls, 4, Lo);
14 net.setTrainSet(trainSetInput, trainSetTarget, true);
15 net.setTrainSimAnnea(100, 100, 10, 0.01, true, 4, 1.0e-12);
16 net.setTrainLevenMar(2000, 1.0e-12);
17 net.Save();
18 Matrix output=net.Run(trainSetInput);
19 double mse=ComputeMse(output, trainSetTarget);
20 // Validation
21 Matrix validSetInput;
22 Matrix validSetInput.Load();
23 Matrix validOutput=net.Run(validSetInput);
24 True mean squared error = 0.000463884
```
Discussion

- Small variations in electrode composition can directly affect cell performance.

- Larger fraction of active materials and a proportional reduction in conductive additive results in reduced cell performance.

- Drying the electrode at room temperature significantly reduced the cell capacity at high C-rates.

- C-rate had negligible effects on cell performance.
Thermal Characterization
Background

- High-temperature operation on Lithium ion batteries induces side reactions and decreases life span.
- Internal shortage can cause thermal runaway, leading to uncontrollable heat generation and potential combustion.
- Battery cooling systems are necessary to keep the battery temperature within the acceptable operating temperature range.

Infrared image of an 18650 battery [10].
Objective

Design a prototype of a phase changing shell for an 18650 battery that allows for heat transfer during charging and discharging to maintain an acceptable operating temperature and prevent it from reaching the point of thermal runaway.

Temperature measurement on an 18650 Li ion battery.
A temperature increase in Li ion battery could cause:

- Increase in chemical reaction, leading to side reactions
- Decrease in efficiency
- Decrease in battery life
- Extreme causes → Battery failure, explosion
Many batteries already feature fuselike structures and several other built-in safety devices. Yet scientists and engineers are working on broader safety strategies that address the characteristics of nearly every battery component.

In rare circumstances, some process could internally or externally short-circuit the battery or subject it to abusive electrical conditions.

An emergency crew arrives on the scene where a UPS 747-400 Boeing cargo plane caught fire due to lithium ion batteries in Dubai on Sept. 5, 2010¹.

¹Source: www.ainonline.com/
Heat Generation Measurement

- Place thermocouple on the surface of battery.
- Obtain data by the NI DAQ.
- Determine convection coefficient by analyzing heat loss over resting phase.
- Determine the total amount of heat generated from temperatures during charge/discharge phases.
- Determine the amount of the phase change material needed.
Energy Balance of the Battery:

\[ \rho V C_p \frac{dT}{dt} = \dot{Q}V - hA(T - T_\infty) \]

Let: \( \theta = T - T_\infty \)

Boundary Conditions: \( \theta = 0 \) at \( t = 0 \)

\[ \theta = \frac{\dot{Q}V}{hA} (1 - \exp \left( \frac{-t}{\rho V C_p hA} \right)) \]
Current and voltage plot for the 18650 battery during the charge and the discharge process.
Current and Temperature difference plot for the 18650 battery.
Heat generation and Temperature difference as a function of time.
Net heat generation vs. time over three charge/discharge cycles.
Convection coefficient can be experimentally determined from rest phase.

Resulting heat transfer rate can be calculated from the energy balance equation and a curve data fitting.

The thickness of phase change material will be determined as a function of the net heat transfer.

Only 8% theoretical change in thermal resistivity between exposed and encased batteries.

Method of phase change determination has still to be verified.
Conclusions
1. This study about Li ion batteries consists on two different approaches, its preparation and safety.

2. In the battery preparation the students learn about the preparation of a coin cell, starting from the electrodes preparation till its assembly and testing.

3. The results obtained from this approach were characterized by a heuristic method, a Neural Network (NN).
5. Current results showed that the trained NN can really predict the main parameters of the cell performance.

6. The second approach was focused on the safety aspect of the 18650 commercial batteries.

7. The analysis focused on the thermal aspect and more specifically on the energy generated.

8. Results from both methods will lead to a better understanding about the performance of the Li ion batteries.
Future Work

1. Develop and characterize a thermal management setup for the 18650 batteries by using a Phase Change Material (PCM).

2. Develop a numerical method that allows to combine the multiple temperature measurements from the cell in order to get a more accurate estimation of the heat generated by the cell.
3. Run an study about the relation between the heat generated during the charging and discharging of the cell with the C-rate at a constant ambient temperature.

4. Increase the number of samples to be used as a training data in the neural network.
References


Acknowledgments

- AggiE Challenge Program, College of Engineering, Texas A&M University
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  - Aashutosh Mistry
  - Chien-Fan Chen
  - Daniel Juárez Robles
- Energy and Transport Sciences Laboratory (ETSL)
  ETSL website: etsl.tamu.edu
Thank You