Development of Cell/Pack Level Models for Automotive Li-Ion Batteries with Experimental Validation

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EC Power
http://www.ecpowergroup.com
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Project ID #
ES120

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Overview

Timeline
• Start date: 5/1/2011
• End date: 4/30/2014
• 33% complete

Budget
• Total project funding: $3.0M
  – $1.5M (DOE)
  – $1.5M (cost share)
• Funding received in FY11
  • $193.6K

Barriers
• Barriers addressed
  – LiB Performance and Lifetime
  – LiB Efficiency
  – LiB Safety
  – Computer tools for design exploration

Partners
• Ford
• Johnson Controls
• Penn State
• NREL
• ORNL

Funding provided by Dave Howell of the DOE Vehicle Technologies Program.
The activity is managed by Brian Cunningham of Vehicle Technologies.
Subcontracted by NREL, Shriram Santhanagopalan Technical Monitor
Project Objectives - Relevance

• Develop an electrochemical/thermal (ECT) coupled model for large-format automotive Li-ion batteries (cells and packs)
• Create a fast & robust tool for realistic geometries (wound or stacked electrode designs)
• Develop a comprehensive materials database
• Integrate ECT3D software with CAEBAT Open Arch. Software
• Aide OEMs and cell/pack developers in accelerating the adoption of large-format Li-ion technology required for EV & PHEV
• Develop a virtual environment to reduce the time required for design, build and test of Li-ion batteries
  – Performance
  – Safety
  – Life
  – Efficiency
• Support DOE CAEBAT activity
## Project Milestones & Activities

### 2011/2012 Milestones Completed

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>M1</td>
<td>Report on initial materials database</td>
</tr>
<tr>
<td>M2</td>
<td>Report/manual for baseline ECT3D software delivered to NREL</td>
</tr>
<tr>
<td>M3</td>
<td>Baseline ECT3D code delivered to NREL</td>
</tr>
<tr>
<td>M4</td>
<td>Updated data for materials database</td>
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<tr>
<td>M5</td>
<td>Report for updated materials database information</td>
</tr>
<tr>
<td>M6</td>
<td>Report for updated materials database information</td>
</tr>
<tr>
<td>Meetings</td>
<td>Meetings with ORNL &amp; other CAEBAT members to give input for the Open Architecture Standard</td>
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<tr>
<td></td>
<td>Battery Safety 2011 – Las Vegas (11/2011)</td>
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<tr>
<td></td>
<td>Presentation to USDrive (12/13/11)</td>
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</tbody>
</table>

### 2012 Milestones in Progress

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>M7</td>
<td>Initial model validation</td>
</tr>
<tr>
<td>M8</td>
<td>Report of safety modeling</td>
</tr>
<tr>
<td>M9</td>
<td>Updated version of ECT3D to NREL w/pack simulation capabilities</td>
</tr>
<tr>
<td>M10</td>
<td>Report for updated materials database information</td>
</tr>
<tr>
<td>M11</td>
<td>ECT3D user interfaces complete</td>
</tr>
<tr>
<td>M12</td>
<td>Report of detailed model validation for ECT3D</td>
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</tbody>
</table>
Approach – Supporting CAEBAT Activity

Task 1: Materials Characterization (PSU)

Task 2: Physico-chemical Models (ECP)

Task 3: Advanced Algorithms (ECP)

Task 4: Experimental Validation (PSU, ECP)

EC Power software: ECT3D

Ford, JCI

Performance

Cycle Life

Safety
Approach – Materials Database

Electrolyte Distribution in a Li-ion Cell Under Discharge

- 4 M
- 1.2 M
- 1 M
- 0.1 M

Nominal conditions for material and battery developers

Modeling parameters needed at low-T, high-T, wide range of chemical compositions and similar conditions of interest for automotive Li-ion batteries and packs.
# Approach – ECT Model Development

## Electrochemical Processes
- electrochemical reactions
- solid state diffusion
- ion transport through electrolyte
- charge transfer

## Thermal Processes
- conservation of thermal energy

\[
\frac{\partial (\rho c_p T)}{\partial t} = \nabla \cdot (\lambda \nabla T) + q
\]

## Heat generation rate

\[
q = \sum_j a_{ij} \bar{I}_y \left( \eta_j + \pi_j \right) - \sum_k \left( <i_k> \cdot \nabla <\phi_k> \right)
\]

## Temperature-dependent physico-chemical properties

\[
\Phi = \Phi_{ref} \exp \left[ \frac{E_{act,\Phi}}{RT} \left( \frac{1}{T_{ref}} - \frac{1}{T} \right) \right]
\]

## Model predictions
- potential and current curves
- temperature history/distribution
- active material utilization
- current distribution

### Understanding thermal phenomena & thermal control has huge impact on
- Battery safety
- Cycle life
- Battery management system
- Cost

### Electrochemical-thermal (ECT) coupling required for
- Internal short circuits
- Thermal runaway
- High power, low-T operation
- Heating from subzero environment
Approach – Computational Challenges

- Develop numerical algorithms to handle:
  1) large electrode size (0.1-1 m²)
  2) multi-layer wound and stacked geometry
  3) ECT couplings, while still maintaining near **real-time** calculations

Compactness Factor (CF) = \[
\frac{\text{Actual Electrode Area}}{\text{Battery Outer Surface Area}} = \begin{cases} 
1 & \text{for coin cells and flat cells} \\
22.5 \text{ or } 32.5 & \text{for 18650 or 26650 cells} \\
60-100 & \text{for pouch cells}
\end{cases}
\]

ThisProposal

ECEC 1999
ECEC 2002
NREL 2009

Negligible thermal effect  |  Significant thermal effect

~100x more challenging

nonuniform current distribution

Cell Capacity (Ah)

Electrode Area (m²)

coin cells  18650  large format batteries

20
Technical Accomplishments

• Development of extensive materials database

• Efficient, electrochemical-thermal coupled large-format cell simulation
  – Performance evaluation and analysis
  – Analysis of active materials utilization
  – Virtual design tool: lower cell cost

• Preliminary validation

• Preliminary safety simulations
  – Full (fast) nail penetration
  – Partial (slow) nail penetration
  – Shorting by metal particle
Material, thermodynamic and kinetic properties for common Li-ion battery materials have been compiled over a wide range of temperature, chemical compositions and SOC.

- Anode AM: graphite, MCMB, LTO
- Cathode AM: MNC, LMO, LFP, NCA, LCO
- Electrolytes: LiPF6 in various solvents
Accomplishments - Validation

- Initial validation efforts at low-T and high C-rate conditions
- Detailed validation efforts currently ongoing
Accomplishments - Performance

3Ah prismatic rolled electrode design – 6C discharge

Performance evaluation and local analysis of active materials utilization over time
Accomplishments - Performance

5-Jelly Roll Cell Design (15 Ah)

- Convective Top & Sides
- Adiabatic Bottom
- $T_{amb} = 300K$
- 1C Discharge

Current density along the electrode length

- @ $t = 100s \rightarrow$ Current density profile determined by material and geometric effects
- @ $t = 3500s \rightarrow$ Current density profile determined by material and geometric effects, local SOC non-uniformity, and thermal effects

Design optimization for active materials utilization
Accomplishments - Safety

Full nail penetration (Fast)

Partial nail penetration (Slow)

Case Study (10Ah prismatic cell)

Only 3-D electrochemical-thermal coupled (ECT) model can completely describe the problem.
Accomplishments - Safety

Full Penetration

Diameter = 0.5 mm

\[
T_{\text{max}} = 180^\circ C \\
T_{\text{avg}} = 34^\circ C \\
T_{\text{max}} - T_{\text{avg}} = 146^\circ C
\]

\[
T_{\text{max}} = 58^\circ C \\
T_{\text{avg}} = 53^\circ C \\
T_{\text{max}} - T_{\text{avg}} = 5^\circ C
\]

\[
T_{\text{max}} = 116^\circ C \\
T_{\text{avg}} = 113^\circ C \\
T_{\text{max}} - T_{\text{avg}} = 3^\circ C
\]

Diameter = 8 mm

\[
T_{\text{max}} = 36^\circ C \\
T_{\text{avg}} = 34^\circ C \\
T_{\text{max}} - T_{\text{avg}} = 2^\circ C
\]

\[
T_{\text{max}} = 52.8^\circ C \\
T_{\text{avg}} = 52.3^\circ C \\
T_{\text{max}} - T_{\text{avg}} = 0.5^\circ C
\]

\[
T_{\text{max}} = 114^\circ C \\
T_{\text{avg}} = 112^\circ C \\
T_{\text{max}} - T_{\text{avg}} = 2^\circ C
\]

Rapid temperature rise caused by electrochemical effects (e.g. nail penetration) can only be predicted with electrochemical thermal (ECT) coupling.
Accomplishments - Safety

Full Penetration

![Graphs showing temperature and voltage changes with nail diameter and time.]

Simultaneous **thermal and electrochemical** results during **safety-related events**

Accomplishments - Safety

Partial Penetration

Temperature (°C) for PD = 0.2

- Maximum temperature (°C) vs. Nail penetration depth (PD) normalized by cell thickness
- Solid Potential for PD = 0.2

Penetrated layers
- Cu foil
- Al foil

Unpenetrated layers
Accomplishments – Safety

Shorting by Metal Particle

- Tab heating is the key mechanism
- 10 Ah, 26 layer stacked cell
- $R_{\text{short}} = 10\, \text{m}\Omega$
- Short in center of layer
- Short in center layer of stack

\begin{itemize}
  \item C-rate in shorted layer
  \item Voltage (V)
  \item Current (C-rate)
  \item Temperature (°C)
\end{itemize}
Accomplishments – Safety

Shorting by Metal Particle

Surface Temperature

Temperature in stack center

Heating greatest in tabs and in metal particle
Collaboration w/Other Institutions

Funding Agency

CAEBAT Program Administrator

Project Lead – Software development and sales, project administration.

Industrial Partner – testing, validation, and feedback

Industrial Partner – testing, validation, and feedback

Academic Partner – materials testing and detailed model validation
Future Work

- More safety simulation of interest to Ford & JCI
- Pack modeling with electrochemical-thermal coupling
- Further and extensive cell and pack validation
- Refined user interfaces
- Life/degradation modeling; optimization of battery usage
- Additional content for materials database
- Blended electrode models (anode & cathode)
- Quarterly review meetings with all team members
Summary

• Good progress in 2011
  – Cell level software development
  – Performance modeling on cell level
  – Preliminary safety modeling of cells
  – Materials database

• Commercial partners (Ford, JCI)
  – Began testing ECT3D in December, 2011
  – Will give expanded feedback during 2012
  – ECT3D is a tool to help
    • Reduce cost, “… by accelerating design processes and system optimization using virtual test bench (software).”
    • Improve safety, “… by understanding the benefits and tradeoffs of various safety technologies.”
    • Improved thermal performances, “… leading to either cost savings or better life.”

• Meeting CAEBAT/DOE goals
  – Helping to accelerate the adoption of automotive Li-ion battery cells & packs
  – Enabling technology for EV, PHEV