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

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Project ID #
ES120

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Overview

Timeline
• Start date: 5/1/2011
• End date: 4/30/2014
• Project 97% complete

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

Budget
• Total project funding: $3.0M
  – $1.5M (DOE)
  – $1.5M (cost share)
  – Fed funds received to date: $1.276M

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
- Develop a comprehensive materials database
- Integrate ECT3D software with CAEBAT Open Architecture Standard (OAS)
- Aid 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

### Recent Milestones Completed

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Description</th>
</tr>
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<tbody>
<tr>
<td>M17</td>
<td>Deliver updated software to partners with OAS compatibility</td>
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<tr>
<td>M18</td>
<td>Complete data of electrode potential curves for series of aged cells</td>
</tr>
<tr>
<td>M22</td>
<td>Additional data for LFP cathode and LTO anode</td>
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<tr>
<td>M23</td>
<td>Report on experimental data for exchange current density</td>
</tr>
<tr>
<td>M24</td>
<td>Report on current and temperature validation</td>
</tr>
<tr>
<td>M26 &amp; 27</td>
<td>Report on life model validation</td>
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<tr>
<td>M29</td>
<td>Report on 3-electrode cell experiments for performance and life</td>
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### Milestones in Progress

<table>
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<tr>
<td>M25</td>
<td>Final report on software</td>
</tr>
<tr>
<td>M28</td>
<td>Deliver final software to partners</td>
</tr>
<tr>
<td>M30</td>
<td>Final report on temperature distribution data</td>
</tr>
<tr>
<td>M31</td>
<td>Final report on OAS compatibility</td>
</tr>
<tr>
<td>M32</td>
<td>Final project report</td>
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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

Data, Cycled Number

Discharge Capacity (Ah)

Cell Voltage (V)
Approach – Materials Database

Tested temperature range for materials

-30°C

100°C

Anode Materials:
• Graphite (blended natural/synthetic)
• LTO

Cathode materials:
• NCM
• LFP
• LMO
• LCO

Electrolyte Concentration

Electrolyte distribution in a Li-ion cell under discharge

Data collected for electrolyte concentrations ranging from 4M to 0.1M

-30°C 100°C

Thousands of coin cells

• Massive undertaking spanning length of project
• High quality material properties lead to validated results for large format cells and packs

-\[ D_s = f(T, x) \]
-\[ \text{EIS for } i_o = f(T, x, c_e) \]

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

### Heat generation rate
\[
q = \sum_j a_j \tilde{I}_j \left( \hat{\eta}_j + \eta_j \right)
- \sum_k \left[ <i_k> \cdot \nabla <\phi_k>^k \right]
\]

### Temperature-dependent physico-chemical properties
\[
\Phi = \Phi_{ref} \exp \left[ \frac{E_{act,\Phi}}{R} \left( \frac{1}{T_{ref}} - \frac{1}{T} \right) \right]
\]

### 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
- Safety simulations
- Thermal runaway
- High power, low-T operation
- Heating from subzero environment
Technical Accomplishments

• Completed data acquisition for materials database
• Validated efficient, electrochemical-thermal (ECT) coupled large-format cell simulation
  – Performance and active materials utilization
• Validated temperature- and design-dependent life model
  – LFP/graphite and NMC/graphite
  – User-defined load profile and thermal conditions
• Validated safety model
• ECT-coupled pack model
• Demonstrated co-simulation with OAS
• Software commercially available
Direct measurement and validation of in-situ current density of a large-format Li-ion battery; ensuring current uniformity is critical for utilization of active material, directly effecting energy density (up to 50%)
Accomplishments – Validation/Performance

In-situ Temperature Distribution

- Effects of Ambient Temperature
- Distribution Over Radius

• In-situ temperature measurement within Li-ion battery
• Data acquired over wide-ranging temperature, C-rate, and thermal boundary conditions
• Validation ongoing

Direct measurement and validation of in-situ temperature distribution
Accomplishments – Validation/Life

Commercial LFP/Graphite Cells

CC Cycling @ 25°C and 45°C

25°C

1C CC cycling at 25°C (symbols are experimental data)

C/10 discharge test at
Month
0 1 3 6 9 12 (4598 cyc)

Voltage (V)
0 2.6 2.8 3 3.2 3.4 3.6
Capacity (mAh)
0 500 1000 1500 2000 2500

45°C

1C CC cycling at 45°C (symbols are experimental data)

C/10 discharge test at
Month
0 1 3 6 9 12 (5017 cyc)

Voltage (V)
0 2.6 2.8 3 3.2 3.4 3.6
Capacity (mAh)
0 500 1000 1500 2000 2500

A123 ANR26650M1-B: Graphite-LFP high power cell
Data from Safari & Delacourt, JES, 258(5) A562, 2011

On-field relevant cycling at 25°C
- Commercial LFP/graphite cell
- Internal life data

Complex Cycling at Room Temperature

- On-field relevant cycling at 25°C
- Commercial LFP/graphite cell
- Internal life data

On-field relevant life cycling of commercial Li-ion cells successfully captured with model at different temperatures; all life models are mechanism-based and valid under wide operating conditions without calibration.
Accomplishments – Validation/Life

NMC/Graphite Cells

• CC cycling at 50°C, 5C-rate
• NMC/graphite cell
• In-house data obtained using 3-electrode cell
• Use of individual electrode potentials for more rigorous validation of life mechanisms in models

Degradation mechanisms in each electrode validated using 3-electrode cell
Accomplishments – Safety/Validation

**Commercial Cell External Short**

- External short of one cell within commercial pack
- Dimensionless current, voltage, and temperature data shown on the left
- Good agreement between data and simulation (temperature within ~ 10%)
- Maximum temperature reached during shorting process can be used to assess safety of design

*Software developed can be used to assess the safety of commercial large-format batteries*
Accomplishments – Safety

ECT3D is used routinely for safety evaluation of large-format cells and safety-conscious designs

- Software gives coupled electrochemical-thermal response of the cells during nail penetration events
- Time scale and locality of heating dictate ability of safety designs to maintain cell safety
  - 5mm nail: short time scale, local heating
  - 20mm nail: long time scale global heating

Safety Simulations in ECT3D

Maximum Temperature During Nail Penetration

Nail Penetration with Coated Phase-change (PC) Material

Physics of Shorting During Nail Penetration
Accomplishments – Other

Other routine uses of software: **pack thermal management design, safety evaluation of large-format cells and safety-conscious designs, and designing batteries with optimal power and energy tradeoff**

Design of pack thermal management

Mixed Electrode Model

Similar results shown in literature: Gallagher et al. JPS 196 (2011) 9702-9707

- Above example shows mixed electrode model used to improve low SOC power via blended NMC/LFP mixture
ECT3D Coupled to Dakota Using OAS

- ECT3D successfully coupled to Dakota optimization software via OAS
- Design optimization demonstrated below
- ECT3D can be coupled to other softwares (e.g. industry internal or other 3rd party) via OAS

ECT3D has been successfully coupled to other software via OAS
Accomplishments – Publications

- Shaffer, C.E. and Wang, C.Y., “Thermal Management for Start-up of Li-Ion Batteries,” 222nd Meeting of The Electrochemical Society (PRiME 2012), Honolulu, HI, October 7-12, 2012
Collaboration w/Other Institutions

Funding Agency

CAEBAT Program Administrator

Project Lead – Software development and sales, project administration.

Industrial Partner – testing, validation, and feedback

Academic Partner – materials testing and detailed model validation

Open Architecture Software

Ford

Johnson Controls

Penn State
Future Work

• **Wrap up final deliverables for this project**
  – M25: Final report on software
  – M28: Deliver final software to partners
  – M30: Final report on temperature distribution data
  – M31: Final report on OAS compatibility
  – M32: Final project report

• **Outside of this project**
  – Pack-level safety
  – Abuse simulation
  – Refined life models
• Last year’s review did not include an individual presentation from our team (CAEBAT overall project presentation/review was given by NREL)
Summary

• All main project goals have been met
  – Development of ECT-coupled cell and pack model
  – Materials database for commercially relevant materials, accurate over wide-ranging T, c_e, SOC, etc.
  – Validated prediction of performance and active material utilization
  – Validated safety models
  – Validated life models

• Commercial partners (Ford, JCI)
  – Have been using updated models in-house for several years
  – Have given invaluable feedback and helped validate model

• Software is commercially available

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