Energy Storage R&D

Computer-Aided Engineering for Electric Drive Vehicle Batteries (CAEBAT)

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### Overview

This presentation covers two related topics: CAEBAT Project and NREL battery modeling work under CAEBAT.

### Timeline

- Project start date: April 2010
- Project end date: Sept 2014
- Percent complete: 15%

### Barriers – Batteries

- Cost and life
- Performance and safety
- Slow prototype-driven design cycles for materials, cells and packs
- Lack of validated battery computer-aided engineering tools suitable for non-expert use

### Budget

- Funding received in
  - FY10: $3.5M ($3.0M for subcontracts)
  - FY11: expected $3.5M ($2.5M for subcontracts)

### Partners

- ORNL
- LBNL
- ANL
- SNL
- INL
- LLNL
- Colorado School of Mines

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Funding provided by Dave Howell, Office of Vehicle Technologies (VT). Activity managed by Brian Cunningham, Vehicle Technologies Program.
Relevance – Need for Better Design Tools

• Computer-aided engineering (CAE) tools are widely used in many industries to speed up the product development cycle and reduce the number of build-and-break steps.

• In fact, use of CAE tools has enabled automakers to reduce product development cost and time while improving the safety, comfort, and durability of the components and the vehicles they produce.

• However, there are no mature CAE tools for the design and commercial development of electric drive vehicle batteries.

• Although there are a number of battery models in academia, national labs, and industry, they either
  – Include relevant physics details, but neglect engineering complexities, or
  – Include relevant macroscopic geometry and system conditions, but use too many simplifications in fundamental physics

• There are a number of custom battery codes available; however, they all require expert users.
Battery CAE capabilities need to be further developed to accelerate the development of batteries.

In previous years, under DOE funding, national laboratories and universities have developed several tools for electrothermal, electrochemical, and abuse reaction modeling of lithium-ion batteries.

The concern has been that they were not all integrated and additional tools were needed.

In April of 2010, the DOE VT Energy Storage Program initiated the multi-year CAEBAT activity to develop design tools and an open architecture software framework that will enable disparate models to interface with each other.
The objective of CAEBAT is to incorporate existing and new models into design suites/tools with the goal of shortening design cycles and optimizing batteries (cells and packs) for improved performance, safety, long life, and low cost.

- The software suite will include material properties, electrode design, pack design for thermal management purposes, load profiles, and aging data as input, and could greatly speed up the design of new batteries and provide critical guidance to developers.
Objectives – NREL CAEBAT Tasks

- As project coordinator, NREL supports DOE in establishing the CAEBAT programmatic activities and objectives.
  - Provide input/documents for the CAEBAT project plan
  - Coordinate activities among national laboratories
  - Support industry and universities through a competitive process to develop battery CAE software tools
- Enhance and further develop NREL’s existing electrochemical, thermal, abuse reaction, and internal short circuit models for use by CAEBAT participants

<table>
<thead>
<tr>
<th>Model</th>
<th>Length Scale</th>
<th>Geometry</th>
<th>Physics / Application</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electro-thermal (FEA) &amp; Fluid-dynamics (CFD)</td>
<td>μm → mm → m</td>
<td>1-D, 2-D, &amp; 3-D</td>
<td>Electrical, thermal &amp; fluid flow, Performance, detailed cooling design, Commercial software (restrictive assumptions)</td>
</tr>
<tr>
<td>Electrochemical-thermal (“MSMD”)</td>
<td></td>
<td>1-D, 2-D &amp; 3-D</td>
<td>Electrochemical, electrical &amp; thermal, Performance, design</td>
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<tr>
<td>Electrochemical-thermal-degradation (“MSMD-life”)</td>
<td></td>
<td>1-D, 2-D &amp; 3-D</td>
<td>Electrochemical, electrical &amp; thermal, Cycling- &amp; thermal-induced degradation, Performance, design, life prediction</td>
</tr>
<tr>
<td>Thermal abuse reaction kinetics</td>
<td>Thermal network, 2-D &amp; 3-D</td>
<td></td>
<td>Chemical &amp; thermal, Safety evaluation</td>
</tr>
<tr>
<td>Internal short circuit</td>
<td>3-D</td>
<td></td>
<td>Chemical, electrical, electrochem. &amp; thermal, Safety evaluation</td>
</tr>
</tbody>
</table>
# List of NREL Milestones

<table>
<thead>
<tr>
<th>Title</th>
<th>Due Date</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>Draft Scope of Work for the CAEBAT program</td>
<td>June 2010</td>
<td>Completed</td>
</tr>
<tr>
<td>Issue Request for Proposals (RFP), review proposals and select industry awardees</td>
<td>December 2010</td>
<td>Completed</td>
</tr>
<tr>
<td>Negotiate and place subcontracts with CAEBAT RFP awardees</td>
<td>June 2011 (Rescheduled)</td>
<td>On Track</td>
</tr>
<tr>
<td>Progress review on the work for the CAEBAT-NREL program</td>
<td>July 2011 (Rescheduled)</td>
<td>On Track</td>
</tr>
</tbody>
</table>
Approach/Strategy

• Based on DOE’s guidance, work with battery community & stakeholders (battery developers, car manufacturers, national laboratories, universities, software companies, etc.) to further refine the scope of the CAEBAT activity:
  – Interact with other national laboratories to understand the capability of existing battery models and other computational capabilities.
  – Interact with industry and universities to understand the scope of their capabilities and eventual needs.
  – Provide input/documents to DOE for defining the CAEBAT project plan.

• Through competitive process, solicit cost-shared proposals from the industry and identify teams to develop battery CAE software tools.

• Perform in-house R&D to enhance and further develop NREL’s existing electrochemical, thermal, abuse reaction, and internal short circuit models for use by CAEBAT participants.
Overall CAEBAT Project
With input from stakeholders, we identified various physics across a wide range of length and time scales that must be addressed, particularly at the pack/vehicle scale.

Physics of Li-Ion Battery Systems in Different Length Scales

- **Electrode Scale**
  - Charge balance and transport
  - Electrical network in composite electrodes
  - Li transport in electrolyte phase

- **Cell Scale**
  - Electronic potential & current distribution
  - Heat generation and transfer
  - Electrolyte wetting
  - Pressure distribution

- **Module Scale**
  - Thermal/electrical inter-cell configuration
  - Thermal management
  - Safety control

- **System Scale**
  - System operating conditions
  - Environmental conditions
  - Control strategy

- **Particle Scale**
  - Li diffusion in solid phase
  - Interface physics
  - Particle deformation & fatigue
  - Structural stability

- **Atomic Scale**
  - Thermodynamic properties
  - Lattice stability
  - Material-level kinetic barrier
  - Transport properties

Active research

Present industry needs
Identified Community’s Expectation for Battery CAE Tools

Accomplishments

- **Address Multi-Scale Physics Interactions**: Integrate different scale battery physics in a computationally efficient manner

- **Flexible**: Provide a modularized multi-physics platform to enable user the choice from multiple sub-model options with various physical/computational complexities

- **Expandable**: Provide an expandable framework to “add new physics of interest” or to “drop physics of low significance or indifference”

- **Validated**: Ensure that the correct equations are solved by performing carefully designed experiments

- **Verified**: The equations are solved accurately
Interacted with Six Other National Laboratories

Accomplishments

- Battery modeling experts from Argonne National Lab (ANL), Sandia National Lab (SNL), Idaho National Lab (INL), and Oak Ridge National Lab (ORNL) visited NREL
- NREL battery researchers visited Lawrence Berkeley National Lab (LBNL), Lawrence Livermore National Lab (LLNL), and ORNL
- The capabilities and potential roles for each lab were identified
- Each lab provided input for the CAEBAT project planning document
- Based on DOE’s guidance:
  - ORNL was funded in FY10 and FY11 to lead Element 4 to develop an open architecture software
  - Other labs were directed to continue any battery modeling work under their existing Advanced Battery Research (ABR) and Batteries for Advanced Transportation Technologies (BATT) Programs
Updated DOE CAEBAT Program Elements

Accomplishments

Assignments for Coordination

- Overall activity: NREL
- Element 1: LBNL
- Element 2: NREL
- Element 3: NREL
- Element 4: ORNL

CAEBAT Program

Element 4: Create Open Architecture Software
- Platform Selection
- Interface Definitions
- Input-Output Formats

Element 3: Develop Pack Models
- CAD Design Layout
- Thermal Models
- Fluid Dynamic Models
- Cost Estimations
- Performance Models
- Pack Management
- Abuse & Safety Models

Element 2: Develop Cell Models
- CAD Design (prismatic cylindrical)
- Thermal Models
- Electrode Design
- Life Models
- Abuse Models
- Structural & Mechanical Models

Element 1: Develop Component Level Models
- Cathode Material Modeling
- Anode Material Modeling
- Electrolyte Modeling
- Electrochemical Couples Modeling
- Abuse Chemistry Modeling
- Separator Modeling

Industry and University Collaborations through RFP

Material-Level Models Developed under BATT and ABR Programs
Initiated Collaboration with Industry

Accomplishments

• Introduced the CAEBAT program at battery conferences and meetings with the United States Advanced Battery Consortium Tech Team
• Prepared a Statement of Work for RFP from industry (car makers, battery developers, battery integrators, universities, and software companies).
  – The purpose was to seek cross-cutting teams to “develop suites of software tools that enable EDV battery community to simulate and design battery packs.”
• NREL issued the CAEBAT RFP on July 30, 2010; many proposals received by September 24, 2010.
• Total DOE/NREL funding is set to be $7.5M over three years with required 50% cost-sharing from participants a project totaling $15 M.
• Source Evaluation Team (SET) consisting of experts from NREL, DOE, and other organizations discussed the proposals during the first two weeks of October 2010.
• By the end of October, the SET reviewed, scored and ranked the proposals; recommended the top three teams for further consideration.
Pending Collaborations with Industry

Accomplishments

• Three industry-led teams were selected for further negotiation with potential awards

• Staff from NREL Contracts and Business Services, with input from three NREL technical monitors, initiated negotiations with the teams to arrive at the subcontracts based on Terms and Conditions dictated by the RFP and the DOE Prime Contract.

• As of the date of preparation of this presentation (3/21/2011), we have resolved all issues except for a few intellectual property (IP) concerns – NREL and the industry teams are determined to resolve the IP issues shortly.
NREL Battery Modeling Under CAEBAT
NREL’s Multi-Scale Multi-Dimensional Model

Relevance

- Introduces multiple computational domains for corresponding length scale physics
- Decouples geometries between submodel domains
- Couples physics in two ways using predefined inter-domain information exchange
- Selectively resolves higher spatial resolution for smaller characteristic length scale physics
- Achieves high computational efficiency
- Provides flexible & expandable modularized framework
We Selected These Cell Designs for Demonstrating MSMD Model Utility

<table>
<thead>
<tr>
<th>Case</th>
<th>Description</th>
<th>$L_x$ [mm]</th>
<th>$L_y$ [mm]</th>
<th>$L_z$ [mm]</th>
<th>Tab width [mm]</th>
<th>Tab configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>ND</td>
<td>Nominal design</td>
<td>200</td>
<td>140</td>
<td>7.5</td>
<td>44</td>
<td>Adjacent tabs</td>
</tr>
<tr>
<td>CT</td>
<td>Counter tab design</td>
<td>200</td>
<td>140</td>
<td>7.5</td>
<td>44</td>
<td>Counter tabs</td>
</tr>
<tr>
<td>ST</td>
<td>Small tab design</td>
<td>200</td>
<td>140</td>
<td>7.5</td>
<td>20</td>
<td>Adjacent tabs</td>
</tr>
<tr>
<td>WS</td>
<td>Wide stack-area design</td>
<td>300</td>
<td>140</td>
<td>5.0</td>
<td>44</td>
<td>Adjacent tabs</td>
</tr>
</tbody>
</table>
MSMD Model Shows Impact of Geometry and Tab Locations on Internal SOC Imbalance (Cell with wide stack area design is worst)

Accomplishments

All cases under 5C Discharge
MSMD Model Shows Impact of Geometry and Tab Locations on Heat Generation and Temperature

Accomplishments

All cases under 5C Discharge

Single side cooling on top surface
- With $h = 25 \text{ W/m}^2\text{K}$
- At $T_{\text{amb}} = 25^\circ\text{C}$

- Similar average temperatures: ND, CT, ST
- Smaller $\Delta T$ at CT
- Larger $\Delta T$ at ST
- Heat generation is highest with WS, but the average $T$ at the End of Discharge (EOD) is lowest

Total Heat Generation

Temperature
Developed Battery Model for Spirally Wound Cells

**Spirally Wound Cell:**
- One pair of wide current collector foils
- Two pairs of wide electrode layers
- Complex electrical configuration

**Stacking process:** Forming a pair between inner electrodes

**Winding process:** Forming a second pair between outer electrodes

**Accomplishments**
- One pair of wide current collector foils
- Two pairs of wide electrode layers
- Complex electrical configuration
The MSMD Model Showed the Larger the Number of Tabs the better the Thermal Performance

Accomplishments

**Temperature comparison**

at 5 min discharge

\[ T - T_{avg}[^\circ C] \]

- **\( \Delta T \)**

- **3.25°C** for 2 tabs

- **0.78°C** for 5 tabs

- **0.37°C** for 10 tabs

- **0.19°C** for Continuous tab
Collaborations and Partnerships

- Collaborating with other national labs to add to the portfolio of capability for CAEBAT
  - ORNL (open architecture software)
  - LBNL (material and electrode models)
  - ANL (material, degradation and cost models)
  - SNL (material safety database and models)
  - INL (electrolyte and degradation models)
  - LLNL (safety modeling)

- Pending cost-shared subcontracts with three industry teams (in negotiations) to develop battery CAE design tools

- Colorado School of Mines – *integrated general chemistry solver for charge transfer and side reactions in Li-ion*


Future Work: Battery CAE

- Finalize negotiations with the three industry teams to execute subcontracts per RFP terms
- Plan kick-off meetings with each CAEBAT-RFP project team to start work
- Finalize the CAEBAT project plan
- Interact with ORNL on the open architecture software
- Finalize roles of other national labs
- Integrate various models in one single platform for industry use
- Perform bottom-up model validation study
- Enhance physics of various models
- Incorporate enhanced solver capabilities and solution schemes
- Hold a conference on Computer-Aided Engineering and Modeling for Automotive Batteries
Summary: Computer-Aided Engineering for Batteries

- Computer-aided engineering (CAE) tools have been widely used by many industries to design products in a shorter amount of time and with lower cost.
- In April 2010, DOE initiated a new program activity (called CAEBAT) to incorporate existing and new battery models into software modeling suites/tools to shorten design cycle and optimize batteries (cells and packs) for improved thermal uniformity, safety, long life, low cost.
- NREL was assigned to coordinate the program with other national labs.
- NREL issued a RFP ($7.5M for 3 years, plus cost share) and screened three industry teams for further negotiations – pending IP issues.
- NREL has been enhancing and further developing its battery models to support CAEBAT program participants.
Technical Back-Up Slides
**MSMD: Extending Beyond Porous Electrode Model**

**Charge Transfer Kinetics at Reaction Sites**

\[
j_{Li} = a_i i_s \left\{ \exp \left[ \frac{a_i F}{RT} \eta \right] - \exp \left[ -\frac{a_i F}{RT} \eta \right] \right\}
\]

\[
i_0 = k (c_e)^{a_s} (c_{s,max} - c_{s,e})^{a_s} (c_{s,e})^{a_s} \eta = (\phi_s - \phi_e) - U
\]

**Species Conservation**

\[
\frac{\partial c_i}{\partial t} = \frac{D_i}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial c_i}{\partial r} \right)
\]

\[
\frac{\partial (\varepsilon_e c_e)}{\partial t} = \nabla \cdot \left( D_e^{\text{eff}} \nabla c_e \right) + \frac{1}{F} j_{Li} - \frac{i_s}{F} \nabla t^s
\]

**Charge Conservation**

\[
\nabla \cdot \left( \sigma^{\text{eff}} \nabla \phi_s \right) - j_{Li} = 0
\]

\[
\nabla \cdot \left( \kappa^{\text{eff}} \nabla \phi_e \right) + \nabla \cdot \left( \kappa_D^{\text{eff}} \nabla \ln c_e \right) + j_{Li} = 0
\]

**Energy Conservation**

\[
\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + q'''
\]

\[
q''' = j_{Li} \left( \phi_s - \phi_e - U + T \frac{\partial U}{\partial T} \right) + \sigma^{\text{eff}} \nabla \phi_s \cdot \nabla \phi_s + \kappa^{\text{eff}} \nabla \phi_e \cdot \nabla \phi_e + \kappa_D^{\text{eff}} \nabla \ln c_e \cdot \nabla \phi_e
\]

- Pioneered by Newman’s group (*Doyle, Fuller, and Newman 1993*) – Dualfoil
  (cchem.berkeley.edu/jsngroup/fortran_files/Intro_Dualfoil5.pdf)
- Captures *lithium diffusion dynamics and charge transfer kinetics – porous media*
- Predicts *current/voltage response* of a battery
- Provides design guide for thermodynamics, kinetics, and transport across electrodes

Difficult to resolve *heat* and *electron current* transport in large cell systems
Temperature Imbalance at End of Discharge

Cooling Surface

Bottom Surface

ND

CT

ST

WS

\( T_{\text{avg}} = 48.1^\circ \text{C} \quad \Delta T = 4.3^\circ \text{C} \)

\( T_{\text{avg}} = 48.0^\circ \text{C} \quad \Delta T = 2.9^\circ \text{C} \)

\( T_{\text{avg}} = 48.5^\circ \text{C} \quad \Delta T = 5.3^\circ \text{C} \)

\( T_{\text{avg}} = 44.7^\circ \text{C} \quad \Delta T = 6.0^\circ \text{C} \)
Number of Tabs Impact Performance

Discharge kinetics rate comparison
in the inner electrode pair at 5 min

\[ \frac{\Delta i''}{i''_{avg}} \]

- **2 tabs**: 32.2%
- **5 tabs**: 6.6%
- **10 tabs**: 2.2%
- **Continuous tab**: 0.2%