Development of Computer-Aided Design Tools for Automotive Batteries

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Date: June 17, 2014

Project ID # ES119

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Overview

Timeline

• Start – June 2011
• Finish – Dec 2014
• 75% Complete

Barriers

• Barriers
  a) Lack of validated computer-aided engineering tools for accelerating battery development cycle
  b) Complexity of multi-scale, multi-physics interactions

Targets

• Targets – shorten time and cost for design and development of EDV and HEV battery packs

Budget

• Total project funding: $7.1 M
  —DOE - $ 3,540 K
  —Contractor – $ 3,540 K
• Funding received
  —FY 12: $ 1,488 K (6/11 – 12/12)
  —FY 13: $ 1,267 K (1/13 – 12/13)
  —Total: $2,755 K
• Funding for FY 14
  —$785 K

Partners

• GM : End user requirements, verification/validation, project management
• ANSYS : Software dev. and commercialization
• ESim : Cell level sub models, life model
• NREL : Technical monitor

Project Lead: GM R&D Center

Funding provided by Dave Howell of the DOE Vehicle Technologies Program.
The activity is managed by Brian Cunningham of Vehicle Technologies.
Subcontracted by NREL, Gi-Heon Kim Technical Monitor
**Project Relevance/Objectives:** faster design cycles and optimize batteries (cells and packs) for improved performance, safety, life, and low cost.

- **Ability to provide trade off studies between various cooling concepts and the battery pack life.**
<table>
<thead>
<tr>
<th>Month /Year</th>
<th>Milestone or Go/No-Go Decision</th>
<th>Status</th>
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</thead>
<tbody>
<tr>
<td>Feb-2013</td>
<td><strong>Go/No-Go decision:</strong> Deliver the cell level simulation tool. The cell level model includes three sub models and a scale coupling based on MSMD approach.</td>
<td>Complete</td>
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<tr>
<td>June-2013</td>
<td><strong>Milestone:</strong> Validation of the cell level model. Deliver the first pack level model. The pack level model includes a system level capability with reduced order models (ROM).</td>
<td>Complete</td>
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<tr>
<td>Sept-2013</td>
<td><strong>Milestone:</strong> System level simulation software tool was delivered. LTI (Linear Time Invariant) system level ROM model approach has been validated in comparison with the full field simulation results.</td>
<td>Complete</td>
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<td>Dec-2013</td>
<td><strong>Go/No-Go decision:</strong> Official public release of ANSYS (version 15) that includes user defined electrochemistry models that allows user to apply their own models while utilizing FLUENT’s battery framework.</td>
<td>Complete</td>
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<tr>
<td>Jan-2014</td>
<td><strong>Milestone:</strong> System level model without ROM was completed and validated compared to the full field simulation and the test data. Demonstrated System simulations for US06 drive cycle. Demonstrated LTI ROM for US06 drive cycle.</td>
<td>Complete</td>
</tr>
<tr>
<td>Dec-2014</td>
<td><strong>Milestone:</strong> Develop CAE process automation for the pack level simulations. Implement cycle life and abuse models. Incorporate NREL’s multi-particle model. Incorporate the Open Architecture Software interface. Deliver the final pack level design tools.</td>
<td>On track</td>
</tr>
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Project Approach

Cell Level Model (Full field simulation)
- Full field simulation based on CFD and electrochemistry model
- Cell level performance including various cooling concepts

System Level Model
- Construct a “linear” or “non-linear” system simulation model from the full pack simulation model

Reduced-Order Models
- Reduced order models for flow and thermal analysis at the pack level

Pack Level Model
- Co-simulation

Strategy is to offer a wide range of methods allowing analysts to trade off computational expense vs. resolution
ABDT is the “umbrella” over all capabilities, including the graphical user interface (UI) that automates/customizes battery simulation workflow, leveraging ANSYS commercial products.
The ANSYS Battery Design Tool (ABDT) has been developed by utilizing the ANSYS Workbench Framework. This framework facilitates the integration of existing applications with external tools to create a seamless workflow.

Model validation is completed for the cell level and module level and is on-going for the production pack level.

Physics based cycle life model has been developed based on a P2D model for the LG cell and a simpler version of equivalent-circuit model (ECM) was derived for a potential cycle life model.

NREL has developed a udf (user defined function) for multiple particle/multiple active material models for GM team.

Linear ROM model developments are on target.

LTI system level model approach has demonstrated for practical simulations of the entire pack for both air and a liquid cooling.

Explored the non-linear ROMS such as POD/DEIM (Proper Orthogonal Decomposition / Discrete Empirical Interpolation Method) for simulating nonlinear realistic battery packs.
Validation of CAEBAT Tools

Cell/Module Simulation

Cell Simulation

Module Simulation

Pack/Module Simulation

System Level Simulation

System model without ROM

Completed for Cell and Module level

Completed for System model

System model with ROM

On target

Liquid Cooling
To validate the system level models with ROM models.

To validate for both full field and the system level simulation.

To validate for system level simulations.
A 24 cell module validation test set up for full field simulation against test data for high-frequency pulse charge-discharge.
Validation for 24 Cell Module

Full Field Simulation Prediction

Measurement

Maximum difference between the prediction and the measurement is within 1 °C.
System Simulation for 24 Cell Module

ABDT User Interface

Generate module and pack model automatically

Electric Circuit

Thermal Circuit
Validation of System Simulation

Test data for average battery temperature

Prediction

0.3°C

1 sec pulse (3.5 C-rate) at 50% SOC

System simulation without ROM reproduced electric and thermal characteristics which are comparable to the test data
Validation of System Simulation for US06 drive cycle

Test data for average battery temperature

Temperature (°C)

Heat generation rate

10 W

Test data for US06 drive-cycle

Prediction
LTI ROM System-Modeling approach for Battery Thermal Simulation

- USO6 drive cycle
- Current profile for USO6
- Terminal Voltage
- SOC
- Heat Generation
- Cell Temperature
- LTI ROM System-Modeling approach for Battery Thermal Simulation

- HPPC Data
- ECM Fitting
- Battery Model
- ROM Model

hybrid pulse power characterization
Comparison between the model and the test data for US06 Drive-Cycle

Test data for US06 drive-cycle

- Foam side temperatures
  - \( \Delta T_{\text{max}} = 0.4^\circ C \)
  - \( \Delta T_{\text{max}} = 0.3^\circ C \)

- Cooling fin side temperatures
  - \( \Delta T_{\text{max}} = 0.7^\circ C \)
  - \( \Delta T_{\text{max}} = 0.7^\circ C \)

SOC vs Time (s)

Voltage, V vs Time (s)
GM has interacted with all the team members, ANSYS, ESIM, ORNL, and NREL.
Last couple years we had weekly progress meetings with ANSYS, ESIM and NREL.
FY 2014, we has planned to have bi-weekly meetings to check the progress.
GM team has provided 4 Quarterly reviews each year to NREL and DOE.
Future Work

Remainder of FY14

— Thermal abuse/runaway model has been developed and will be implemented in the 2nd Q to handle the thermal propagation in the pack.

— Practical cell cycle life models have been defined and it is planned to be included in 3rd Q. The physics based cycle life model will be implemented 4th Q.

— Complete workflow automation for LTI/LPV ROM process.

— Implement models for multiple active/particle materials.

— Pack level verification, validation, and demonstration.

— Complete battery-specific graphical user interface (ABDT)

— Complete a standard data-exchange interface based on specifications from the OAS Workgroup
Summary

• **Several software deliverables for the cell level tools.**
  - NREL’s MSMD framework is implemented in FLUENT with three electrochemistry sub-models, 2Q 2013.
  - Cell level validation was completed, 3Q 2013.
  - Developed user defined electrochemistry models that allows user to apply their own models while utilizing FLUENT’s battery framework, 4Q 2013.
  - The major release of FLUENT Version 15 in December 2013 contains NREL’s MSMD battery model further developed jointly by GM and ANSYS.

• **First pack level software tool was delivered to GM, NREL, and ESim**
  - Auto electrical connection by detecting the cell configurations in the pack.
  - Code is completely parallelized, 2Q 2013.

• **Cycle life test completed with 30% capacity fade.**
  - Cycle life test at an elevated temperature is in progress and to be completed in 4Q 2014.
  - Physics based cycle life model has been developed and to be implemented in 4Q 2014.

• **Pack level validation is completed for a 24 cell module.**
  - Full field simulation was validated in 4Q 2013.
  - System level model was completed and validated compared to the full field simulation and the test data and comparisons are satisfactory 1Q 2014.
  - LTI system level ROM model approach has been validated in comparison with the full field simulation results 2Q 2013.
  - Demonstrated for USO6 driving cycles and validated in 4Q 2013 and 1Q 2014.
Sustainable Software Tool (CAEBAT)

Support of DOE CAEBAT

*The automotive industry requires CAE design tools that include the following capabilities.*

- **Modular:**
  - Integrate physics and chemistry in a computationally efficient manner.
- **Provide Flexibilities:**
  - Provide a platform to enable various simulation strategies.
- **Provide Expandable Framework:**
  - Enable future users to easily add new physics of interest.
  - OAS-compatible.
- **Validated:**
  - Ensure model predictions agree with experimental data by performing carefully designed experiments.
- **Easy to use**
Technical Back-Up Slides
Why Multi-Particle Model?

**Multiple Particle Model Uses**

- Two-cathode and Two-anode cells are going into *production vehicles*.
- OCVs of two cathode materials, their diffusion mechanisms are different causing **highly nonlinear HPPC response** that even 6P or 8P models were not able to capture.
- Developing an **equivalent single electrode** is turning out to be a challenge for certain chemistries.
- Diffusion coefficients and other time constants are functions of SOC, charge vs. discharge.
- **Physics-based degradation models** for multiple particle models need to be developed – long term.
- **Battery cell manufacturers** are interested in evaluating effect of particle size distribution (skewness, variance) on material utilization, performance (P/E ratio) using virtual methods – experimental techniques take years to assess.
Electrode Particle Morphology
Implementation of NREL’s Multi-particle Model in ANSYS/Fluent using MSMD Protocol

- **ANSNS**: It will be a demonstration of expandability and flexibility of the model architecture that ANSYS/Fluent adopted in the project.

- **GM**: GM is interested in using the model with multiple particle, multiple active material features. GM CAE and Battery Algorithms teams are ready to apply these models.

- **DOE/NREL**: NREL’s developments can be quickly available to EV industries through CAEBAT program products.

- **Public Benefit**: This would be a good success story of delivering expertise in national lab to a direct use of EV industry using the DOE’s CAEBAT product outcomes.
Reformulation of Deshpande’s model

• The model equations in original form

\[
\frac{dQ}{dN} = 2B AL_{SEI}^a \left(1-CN\right)^{m} - B \left(1 + 2l_{cr} \rho_s a_0 \right) \frac{1}{2} K_{th} \left(N\right)^{-1/2} - 2 B A \sum_{i=1}^{N-1} \left[1-C \left(N-i\right)\right]^{m} \frac{1}{2} K_{th} \left(N-i\right)^{-1/2}
\]

\[
A = l_{cr} \rho \left[ \frac{\pi a}{15 \left(1-v\right)} \right]_{E} \left[ F D_{s} \right]
\]

\[
\sigma_{0,\text{max}} = -\frac{1}{15 \left(1-v\right)} \left[ i R_{c} \right] \Omega
\]

\[
B = \frac{n_{\text{SEI}} F \rho_{\text{SEI}} 4 \pi R_{s}^{2}}{3600 \left[\text{s} \cdot \text{hr}^{-1}\right] M_{\text{SEI}} Q_{0}}
\]

\[
C = -\frac{2-m}{2} k \left[ \sigma_{0,\text{max}} b \sqrt{\pi a_{0}} \right]^{m} \left(\frac{m}{2}\right)
\]

The parameter values in Deshpande’s model vary with materials and electrode designs; so a life model should involve the validation of the capacity fade equation

• The reformulated model equations

\[
\frac{dQ}{dN} = b_1 \left(1 - b_2 N\right)^{-b_3} - b_4 \left(N\right)^{-1/2} - b_5 \sum_{i=1}^{N-1} \left[1-b_2 \left(N-i\right)\right]^{b_3} \left(N-i\right)^{-1/2}
\]

\[
\text{where } b_1 = 2B AL_{SEI}^a, \quad b_2 = C, \quad b_3 = \frac{m}{m-2}, \quad b_4 = B \left(1 + 2l_{cr} \rho_s a_0 \right) \frac{1}{2} K_{th}, \quad b_5 = B A K_{th}
\]

The parameter vector is defined as \( \mathbf{b} = [b_1, b_2, b_3, b_4, b_5] \)

The capacity fade equation can be expressed as \( \frac{dQ}{dN} = f(\mathbf{b}, N) \)
The extrapolatability of Deshpande’s model

To check the extrapolatability of Deshpande’s model, there should be more OPCAP data points during the initial cycling stage (i.e., the first 500 cycles) than during the later stage (i.e. >500 cycles); therefore, we generated synthetic data with random noise (± 0.01 in fractional capacity) where nine OPCAPs (BOL, cycle #10, 20, 50, 100, 200, 300, 400, and 500) were included during the first 500 cycles.

Fit Deshpande’s model to the synthetic capacity data at “finished cycles”

Run the model with the parameter values obtained in the previous step and extend the simulation to the “future cycles”

Compare the model predictions and the synthetic data values at the “future cycles”

The synthetic data with noise
The Periodic HPPC measurements

- Before each OPCAP check, the HPPC of the cell was measured.
- In each HPPC, 9 pulses were made at different SOC, and the first 8 pulses were chosen to be used for model validation.

The HPPC voltage profile

- The 1st pulse
- The 2nd pulse
- The 3rd pulse
- The 4th pulse
- The 5th pulse
- The 6th pulse
- The 7th pulse
- The 8th pulse

The HPPC voltage profile
Fitting ECM to HPPC at BOL

The 1st pulse

The 2nd pulse

The 3rd pulse

The 4th pulse

The 5th pulse

The 6th pulse

The 7th pulse

The 8th pulse
Fitting ECM to HPPC at 1000th cycle

The 1st pulse

The 2nd pulse

The 3rd pulse

The 4th pulse

The 5th pulse

The 6th pulse

The 7th pulse

The 8th pulse
Fitting ECM to HPPC at 2000\textsuperscript{th} cycle

The 1\textsuperscript{st} pulse

The 2\textsuperscript{nd} pulse

The 3\textsuperscript{rd} pulse

The 4\textsuperscript{th} pulse

The 5\textsuperscript{th} pulse

The 6\textsuperscript{th} pulse

The 7\textsuperscript{th} pulse

The 8\textsuperscript{th} pulse
1. Taeyoung Han, Gi-Heon Kim, Lewis Collins, “Multiphysics simulation tools power the modeling of thermal management in advanced lithium-ion battery systems,” ANSYS Quarterly magazine "Advantage", 2012


8. Ramesh Rebba, Justin McDade, Shailendra Kaushik, Jasmine Wang, Taeyoung Han, ”Verification and Validation of Semi-Empirical Thermal Models for Lithium Ion Batteries ,” to be presented in 2014 SAE World Congress.