Development of Computer-Aided Design Tools for Automotive Batteries

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General Motors R&D Center
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Project ID # ES119

This presentation does not contain any proprietary, confidential, or otherwise restricted information
Overview

Timeline

• Start – June 2011
• Finish – May 2014
• 20% Complete

Barriers

• Barriers
  a) Material properties and cell structures are proprietary and difficult to obtain
  b) Complexity of multi-scale, multi-physics interactions

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

Budget

• Total project funding: $7.2 M
  —DOE - $ 3,600 K
  —Contractor – $ 3,600 K
• Funding received in FY11
  —$ 369 K
• No funding change

Partners

• GM : End user requirements, verification/validation, project management
• ANSYS : Software development
• 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.
Development of Computer-Aided Design Tools for Automotive Batteries (CAEBAT)

Project Objectives - Support of DOE CAEBAT

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

• **Address Multi-Scale Physics Interactions:**
  — 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.

• **Verify and Validate Models:**
  — Ensure model predictions agree with experimental data by performing carefully designed experiments.
# Milestones

<table>
<thead>
<tr>
<th>Month /Year</th>
<th>Milestone or Go/No-Go Decision</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>June-2012</td>
<td><strong>Go/No-Go decision:</strong> Define end user requirements for the cell level and the pack level design tools. The cell level model includes three sub models that covers the particle and electrode level (P2D), Semi-empirical cell level model (NTGK), and equivalent circuit model (ECM). Demonstrate scale coupling of various sub models by MSMD approach for the cell level. <strong>Milestone:</strong> Deliver the first cell level model.</td>
<td>On track</td>
</tr>
<tr>
<td>June-2013</td>
<td><strong>Milestone:</strong> Validation of the cell level model. Deliver the final cell level simulation tool. Deliver the first pack level model. The pack level model includes a system level co-simulation capability and reduced order models (ROM).</td>
<td>On track</td>
</tr>
<tr>
<td>June-2014</td>
<td><strong>Milestone:</strong> Validation of the pack level model. Develop CAE process automation for the pack level simulations. Deliver the final pack level design tools. Incorporate the Open Architecture Software interface to allow other sub models, material database, physical input parameters, and future sub models.</td>
<td>On track</td>
</tr>
</tbody>
</table>
Approach for Cell Level

Electrode Level
- Electrochemical kinetics
- Solid phase Li diffusion
- Li transport in electrolyte
- Charge conservation & transport

Cell Level
- Electric potential field
- Current density field
- Cell capacity, capacity/power fade
- Cell temperature
- State of Charge
- Coupled with flow and heat transfer for cooling channel design

Scale Coupling (MSMD)

1-D Field Simulation
- Finite Volume Method

Reduced Order Model
- State Variable Model (SVM)
- Preferred Orthogonal Decomposition (POD)

Empirical Model
- Equivalent Circuit
- Current Density (U, Y)

Aging/depredation Abuse

Cost

3D field simulation
- Navier-Stokes solver
- Finite Volume Method

Reduced Order Model
- Linearized model
- Non-liner model

Transfer Function
- Map the field solution to transfer variables

Models are available
To be developed
Approach for Pack Level Simulation

- Strategy is to offer a wide range of methods allowing analysts to trade off computational expense vs. resolution

**Cell Level Model**
- Reduced Order Models for electrochemistry
- Cell level performance including local cooling channels

**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
- Reduced order cell models
- Ability to “expand” results

**Pack Level Model**
- Co-simulation
Sub-models Integrated into the Cell

Electrochemical sub-models relate the local current density to the potential. Cell model couples sub-models to thermal and electrical fields within the cell, integrates over multiple electrode-pairs.

Newman, Li transport model (P2D)

Newman, Tiedemann, Gu, Kim (NTGK)

\[ J = Y(V_p - V_n - U) \]

\[ U = f(DOD,T) \]

\[ Y = g(DOD,T) \]

Equivalent Circuit Model (ECM)
<table>
<thead>
<tr>
<th>Model</th>
<th>Pros</th>
<th>Cons</th>
<th>Potential application area</th>
<th>Further development</th>
</tr>
</thead>
<tbody>
<tr>
<td>P2D</td>
<td>Detailed electrochemistry modeling approach. Solve particle and electrode level including electrolyte</td>
<td>Potential to simulate local detail and cover wide range of cell chemistry</td>
<td>Many physical input parameters and material properties. Difficult to obtain these from the measurements.</td>
<td>Cell design</td>
</tr>
<tr>
<td>NTGK</td>
<td>Semi-empirical approach. 2 key functional parameters, U, Y. Solve electrical potential for the current collectors.</td>
<td>Practical 2-D approach. Non-uniform SOC, heat distribution</td>
<td>Unable to predict cell design changes without testing</td>
<td>Cell/Pack integration</td>
</tr>
<tr>
<td>ECM</td>
<td>Empirical parameter fit from test data. Do not solve electric potential field.</td>
<td>Very simple. computationally very fast</td>
<td>Unable to predict cell design changes without testing</td>
<td>Pack optimization</td>
</tr>
</tbody>
</table>
## Pack Level Strategies

<table>
<thead>
<tr>
<th>Model</th>
<th>Pros</th>
<th>Cons</th>
<th>Potential application area</th>
<th>Further development</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Co-simulation</strong></td>
<td>CFD-based cell models iteratively coupled to network/circuit pack model</td>
<td>Most accurate, no need for ROM-building, Earliest availability for testing</td>
<td>Computational cost (but can exploit periodicity, sampling, module hierarchy to improve over brute force approach)</td>
<td>Totally new designs, validation</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Asynchronous time stepping, Automated user interface</td>
</tr>
<tr>
<td><strong>Transient ROM</strong></td>
<td>Build time-varying cell ROM from CFD, then use in pack-level simulation</td>
<td>Most efficient</td>
<td>Linearized about some particular values, e.g. coolant flow rate, state of health, etc.</td>
<td>Drive cycles, parametric studies</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>ROM algorithms, Storage, Results expansion</td>
</tr>
<tr>
<td><strong>System level model</strong></td>
<td>Construct system level models from the full pack simulation model.</td>
<td>Very fast and efficient</td>
<td>Solution available only at monitored locations. Requires full 3-D pack-level flow/thermal solution.</td>
<td>Battery management system, Drive cycles</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Non-linearity due to variable flow rates</td>
</tr>
</tbody>
</table>
The first cell level tool will include 3 sub-models with a standard battery user interface and an open interface for other sub-models. Cell level verification and validation will be performed after the first cell level tool is available.
Technical accomplishments – Year 1

- End user needs have been defined for the cell level and the pack level design tools. Battery manufacturer’s requirements has been obtained from LG Chem.
- Survey of existing potential cell level models has been completed.
- All three cell-level approaches have been prototyped.
- Simulor-FLUENT co-simulation feature has been prototyped.
- Initial research has been conducted on ROM methods.
- Scale coupling between particle, electrode, and cell levels has been tested based on MSMD approach.
- A test plan and procedure for collecting test data from production cells to validate the cell design tool has been completed.
- CAE capability matrix has been defined for pack level applications in automotive industry.
- Performed monthly progress reviews with NREL and quarterly reviews with NREL and DOE.
Researching Simulation Best-Practice

- P2D particle resolution study (non-uniform radial grid)
- Findings will be built into deliverables, providing automation for non-experts

**10C discharge rate**

![Graph showing Li concentration at solid-electrolyte interface Cs_e, mol/lm^3 vs. r/R for different N and p values.](image)

- N=35, p=1.0
- N=70, p=1.0
- N=30, p=0.9
- N=20, p=0.8
- N=10, p=0.6
ECM was implemented as a sub-model and validated with other results.

NTGK Model implementation

\[
\nabla^2 V_p = -r_p J \quad \text{in} \quad \Omega_p \\
\nabla^2 V_n = +r_n J \quad \text{in} \quad \Omega_n
\]

U and Y are fitting parameters depend on Depth of Discharge (DOD) and Temperature

Current Density Model

\[
\nabla \cdot (\varepsilon_+ \sigma_+ \nabla \phi_+) = +aj \\
\nabla \cdot (\varepsilon_- \sigma_- \nabla \phi_-) = -aj \\
\nj = aY (\phi_+ - \phi_- - U) \quad A/m^3
\]

3-D Finite Volume

Discharge curve
Cell Level Test & Validation by GM

<table>
<thead>
<tr>
<th>Test</th>
<th>Test Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell relaxation test</td>
<td>Environmental Temperature range: -20, -10, 0, 25, 40 Deg C C rate: 0.5C, 1C, 3C and 4C</td>
</tr>
<tr>
<td>Static capacity and HPPC test</td>
<td>Environmental Temperature range: 0, 10, 25, 40 Deg C</td>
</tr>
<tr>
<td>IR thermal imaging</td>
<td>10 to 90% SOC, room temperature, 1C, 3C and 4C</td>
</tr>
<tr>
<td>Cell cyclic life test</td>
<td>Environmental Temperature range: 0, 10, 25, 40 Deg C C rate: 2C, 3C SOC window: 30% to 90%</td>
</tr>
<tr>
<td>Cell Calorimeter</td>
<td>Same test condition cell cycling test</td>
</tr>
</tbody>
</table>

- Cell level validation test for electrical and thermal performance for the cell
- Thermocouple, thermal imaging, calorimeter test to measure the total heat generation and non-uniform heat source
- Cycle life test for aging model
Cell Cycle Life Test Procedure

Test Cells in Thermal Chamber

Temperature Monitor Point

Table 1: Cycle Test Temperature

<table>
<thead>
<tr>
<th>Test</th>
<th>Parameter</th>
<th>Cycle Test Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>2C cycle</td>
<td>Discharge Current</td>
<td>30A  30A  30A  30A</td>
</tr>
<tr>
<td>3C Cycle</td>
<td>Discharge Current</td>
<td>45A  45A  45A  45A</td>
</tr>
</tbody>
</table>

Table 2: Cycle Test Temperature

<table>
<thead>
<tr>
<th>Test</th>
<th>Parameter</th>
<th>Cycle Test Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>2C cycle</td>
<td>Charge Current</td>
<td>12A  20A  30A  30A</td>
</tr>
<tr>
<td>3C Cycle</td>
<td>Charge Current</td>
<td>20A  30A  30A  30A</td>
</tr>
</tbody>
</table>
Pack Level Validation

Pack level test
• Driving cycles
• Environmental temperatures
• Thermocouple location
• Coolant flow rate & temperature
• Cell chemistry

Validation Parameters
• SOC, Cell Voltage, Cell Temperatures
• Coolant flow Temperature in & out
• Total heat generation

♦ Pack level validation test data will be carefully selected from the existing GM battery Test database.
Collaborations

- Project management
- Project lead
- Pack level strategy
- Cell / Pack level verification & validation
- Vehicle level validation under various driving schedules
- math model verification and validation
- Set vehicle requirements for cell and pack design
- Pack level validation
- tests for cell level validations
- flexible frame work for multi-physics models
- cell/pack level simulation capability development
- Process automation & OAS
- Physics based cell aging model for capacity fade and cell life
- Model order reduction methods
- Tool verification and validation
- Project technical direction (Tech monitor)
- Open Architecture Software
Future Work

• Develop model order reduction methods for the pack level
• Extend cell-level models for aging and abuse
• Cell level verification and validation
• Pack level verification, validation, and demonstration
  ✓ Define pack level validation requirements to meet the future capability matrix for pack level CAE performance.
  ✓ Identify suitable existing pack level test in progress or from previous tests (Liquid or Air cooling) performed in GM battery group.
  ✓ Build up the pack level simulation model including meshing and physical boundary conditions, operating conditions.

• Develop battery-specific graphical user interface for workflow automation
• Build a standard data-exchange interface based on specifications from the OAS Workgroup
Summary

• Overall project is on-track to meet all objectives, Year 1 technical progresses are consistent with the plan

• Cell level end user requirements have been defined and completed;
  ✓ Model inputs and outputs, geometry & meshing requirements, performance requirements. Standard input parameters were defined and shared with the OAS Work Group.
  ✓ End user requirements from the battery manufacturer (LG Chem) was obtained. Other battery manufacturers are under consideration.

• Cell level validation test in progress;
  ✓ Cell performance test in progress, cycle life test has been initiated.
  ✓ Two different cell chemistries are chosen for validation (LG Chem, A123).

• Pack level end user requirements have been defined and completed;
  ✓ CAE capability matrix, functionalities, user friendly features, acceptable accuracies and requirements for CPU time & turnaround time.

• Principal remaining efforts and technical risks in the area of pack-level model;
  ✓ Various Pack level simulation strategies are under evaluation.
Technical Back-Up Slides
Porous Electrode Lithium Ion Battery Model

- Positive Electrode:
  \[
  \frac{\partial c_{s,p}(r,t)}{\partial t} = D_{s,p} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial c_{s,p}(r,t)}{\partial r} \right) \\
  \frac{\varepsilon_p}{\partial t} = D_{eff,p} \frac{\partial^2 c}{\partial x^2} + (1 - t_+) a_p j_p \\
  \sigma_{eff,p} \frac{\partial^2 \Phi}{\partial x^2} = a_p F j_p
  \]

- Negative Electrode:
  \[
  \frac{\partial c_{s,n}(r,t)}{\partial t} = D_{s,n} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial c_{s,n}(r,t)}{\partial r} \right) \\
  \frac{\varepsilon_n}{\partial t} = D_{eff,n} \frac{\partial^2 c}{\partial x^2} + (1 - t_+) a_n j_n \\
  \sigma_{eff,n} \frac{\partial^2 \Phi}{\partial x^2} = a_n F j_n
  \]

- Separator:
  \[
  \varepsilon_s \frac{\partial c}{\partial t} = D_{eff,s} \frac{\partial^2 c}{\partial x^2} \\
  \kappa \frac{\partial}{\partial x} \left( \kappa_{eff,s} \frac{\partial \Phi}{\partial x} \right) + \beta \frac{\partial}{\partial x} \left( \frac{\partial \ln c}{\partial x} \right) = 0
  \]

- BV: \[ j_i = 2k_i \left( c_{s,max,i} - c_s(R_{s,i}) \right)^{0.5} c_s(R_{s,i})^{0.5} c_s^{0.5} \sinh \left( \frac{0.5F}{RT} (\Phi_i - \Phi_2 - U_i) \right) \]
$\Phi^+$ and $\Phi^-$ are the potential at the positive and the negative current collectors.

$T$, temperatures are from the cell level domain. No energy equations in the electrode and the particle domain.

$\Phi^+$ and $\Phi^-$ provide to the electrode to compute potentials in the electrode interfaces.

Current is generated from the particle level and applied for the electrode and the cell domain.

Heat source is generated from the particle level (heat of charge transfer and mixing).

Heat source is also added in the electrode region by contact resistance and others.
20-Ah LG Normal Design cell

Modeling with finite element method

Real cell*

Flowchart for distributed pseudo-2D thermal model

Energy balance

\[ \rho C_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q + \sigma_p \nabla \Phi_p \cdot \nabla \Phi_p + \sigma_n \nabla \Phi_n \cdot \nabla \Phi_n \]

Limiting electrical conditions

\[ \nabla \cdot (\sigma_p \nabla \Phi_p) + \frac{i_p}{0.5 \delta_{pcc}} = 0 \quad \nabla \cdot (\sigma_n \nabla \Phi_n) - \frac{i_p}{0.5 \delta_{ncc}} = 0 \]

\[ \frac{1}{HW} \int_{\Omega} i_p dX dY = - \frac{I_{app}}{A_{cc}} \]

\[ \Phi_j = \Phi_j + \Delta \Phi_j \]

Both energy balance and limiting electrical conditions satisfied?

No

Yes, go on to next time step

\[ T_{Test} = T_{Test} + \Delta T \]
20-Ah LG Normal Design cell

- Anode initial SOC: 0.63
- Cathode Initial SOC: 0.41
- End of discharge voltage: 2.5V

Convective heat flux