A Total Li-Ion Battery Simulation Solution (Part 1)*

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*Part 2: Structural Integrity Assessment of a Li-Ion Battery Pack Using Simulation
## A Total Li-Ion Battery Simulation Solution

### Small Scale

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<th>Molecular</th>
<th>Electrode</th>
<th>Cell</th>
<th>Module/Pack</th>
<th>Powertrain</th>
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<td>SEI</td>
<td>Safety</td>
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<tr>
<td>Electro-chemistry</td>
<td>ECM</td>
<td>ECM</td>
<td>ECM</td>
<td>ECM</td>
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<td></td>
<td>CFD</td>
<td>CFD</td>
<td>ROM</td>
<td>ROM</td>
</tr>
<tr>
<td></td>
<td>FEA</td>
<td>FEA</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Large Scale

- Cell: ECM, CFD, FEA
- Module/Pack: ECM, CFD, ROM, FEA
- Powertrain: ECM, ROM
A Total Li-Ion Battery Simulation Solution
Electrode Level - Electrochemistry

- Electrochemical Kinetics
- Solid-State Li Transport
- Electrolytic Li Transport
- Charge Conservation/Transport
- (Thermal) Energy Conservation

Impact of Discharge Rate on Capacity

Temperature Impact on Capacity

Charge Discharge Cycles

Impact of Discharge Rate on Capacity

Temperature Impact on Capacity

Charge Discharge Cycles

X. Hu, S. Lin, S. Stanton, SAE paper 2012-01-0665
Impact of Temperature on Concentration Distribution

Impact of Particle Shape on Capacity

Validation of Reduced Order Electrochemistry

Electrode Level - Electrochemistry

Newman P2D Electrochemistry Model in Fluent (CAEBAT project)

\[ \nabla \cdot (\sigma \nabla \phi_s) - j^{Li} = 0 \]
\[ \nabla \cdot (k \nabla \phi_e) + \nabla \cdot (k_D \nabla \ln c_e) + j^{Li} = 0 \]
\[ j^{Li} = \xi_a i_0 \left\{ \exp \left( \frac{\alpha_a F}{RT} \eta \right) - \exp \left( -\frac{\alpha_c F}{RT} \eta \right) \right\} \]

\[ \frac{\partial (\varepsilon_e c_e)}{\partial t} = \nabla \cdot (D_e \nabla c_e) + \frac{1-t^+}{F} j^{Li} \]
\[ \frac{\partial c_s}{\partial t} = \frac{D_s}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial c_s}{\partial r} \right) \]

Domains
- negative electrode
- separator
- positive electrode
- spherical particles

A system of DAEs are solved for every CFD cells:
- Total number of equations: \((n_{Cs} + 2) \times n_{NE} + 2n_{SP} + (N_{Cs} + 2) \times n_{PE}\)
- Memory requirements: \(N_{cell} \times \{(n_{Cs} + 1) \times n_{NE} + n_{SP} + (N_{Cs} + 1) \times n_{PE}\}\)

Temperature Results Based on Electrochemistry

Current (A) vs. Time (s)

Cell Voltage (V) vs. Time (s)

Tmax (K) vs. Time (s)
Cell Level – Equivalent Circuit Model (ECM)

Battery Equivalent Circuit Model (ECM)

Simulation

Testing

• 28 Cells are connected in a module
• 4 modules are connected to the final configuration

Simulation Results

Battery Pack ECM

Cell Level – ECM Extraction Tool

Voc vs. SOC

Pulse Discharge

Modeling Error
Cell Level – ECM Extraction Tool

ECM Extraction Toolkit

ECM Model Workflow

Module Level – CFD Thermal

Temperature Distribution

Temperature and Pathlines
Motivation of Reduced Order Model (ROM)

CFD as a general thermal analysis tool is accurate.
- Can be computationally expensive for system level analysis

ROM can significantly reduce the model size and simulation time.
ROM is an import tool for system level simulation.
Battery Thermal Behavior via ROM

Type 1: Thermal Network
- Careful calculation and calibration needed
- Accuracy compromises

Type 2: LTI – state space
- Can be as accurate as CFD
- No calibration
LTI ROM for Battery Cooling

1. Create the CFD model
2. Generate step responses
   - Icepak has specialized tools
   - Other CFD codes are fine
3. Extract LTI ROM
   - Use Simplorer
4. Simulate inside Simplorer
LTI ROM gives the same results as CFD. LTI ROM runs in less than 2 seconds while the CFD runs 2 hours on one single CPU.
Module Level – ROM for Thermal

ROM vs CFD

ROM for the Battery Module
SVD+LTI ROM : GM 16 Cell

Test Case

SVD+LTI technology allows for quick temperature distribution calculation in addition to average temperature calculation. Using a heat source from GM, SVD+LTI ROM is applied to the GM 16 cell case.

Heat source used
SVD+LTI ROM for Battery Cooling

1. Create the Fluent CFD model
2. Generate step responses
3. Extract SVD+LTI ROM
   - Use Simpleror
4. Simulate inside Simpleror
SVD+LTI ROM Validation: GM 16
Cell Test Case

CFD (200 sec)

SVD+LTI ROM (200 sec)

CFD (400 sec)

SVD+LTI ROM (400 sec)

CFD (600 sec)

SVD+LTI ROM (600 sec)

CFD (800 sec)

SVD+LTI ROM (800 sec)
### SVD+LTI ROM Statistics for GM 16 Cell Test Case

<table>
<thead>
<tr>
<th>CFD mesh size</th>
<th>3,025,067</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of steps in step response run</td>
<td>180</td>
</tr>
<tr>
<td>Size of matrix $A$</td>
<td>3,025,067×180</td>
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<tr>
<td>Number of snap shots used for SVD calculation</td>
<td>180</td>
</tr>
<tr>
<td>SVD calculation time</td>
<td>4 min 50 sec</td>
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<tr>
<td>SVD calculation memory usage</td>
<td>8.1 G</td>
</tr>
<tr>
<td>SVD+LTI ROM extraction time</td>
<td>5 min</td>
</tr>
<tr>
<td>CFD validation simulation time on single CPU</td>
<td>5 hr</td>
</tr>
<tr>
<td>SVD+LTI ROM simulation time on the same single CPU</td>
<td>a few seconds</td>
</tr>
</tbody>
</table>
SVD+LTI ROM Validation

CFD (10 sec)  

CFD (20 sec)  

CFD (30 sec)  

CFD (40 sec)  

SVD+LTI ROM (10 sec)  

SVD+LTI ROM (20 sec)  

SVD+LTI ROM (30 sec)  

SVD+LTI ROM (40 sec)
## SVD+LTI ROM Statistics for the Test Case

<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>CFD mesh size</td>
<td>12,209,486</td>
</tr>
<tr>
<td>Number of steps in step response run</td>
<td>120</td>
</tr>
<tr>
<td>Size of matrix $A$</td>
<td>12,209,486×120</td>
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<tr>
<td>Number of snapshots used for SVD calculation</td>
<td>60</td>
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<tr>
<td>SVD calculation time</td>
<td>3 min</td>
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<tr>
<td>SVD calculation memory usage</td>
<td>18 G</td>
</tr>
<tr>
<td>SVD+LTI ROM extraction time</td>
<td>5 min</td>
</tr>
<tr>
<td>CFD validation simulation time on six CPUs</td>
<td>20 hr</td>
</tr>
<tr>
<td>SVD+LTI ROM simulation time single CPU</td>
<td>a few seconds</td>
</tr>
</tbody>
</table>
GM Battery Module – ECM
Coupled with ROMs

ECM calculates heat source and sends it to the two ROMs. LTI ROM calculates average temperature and sends it to ECM. SVD+LTI ROM *calculates* temperature distribution.
ROM Results

- LTI ROM calculates average temperature.
- SVD+LTI ROM calculates temperature field.
Temperature Distribution - Animation

Temperature calculated from CFD. 7 hr simulation time with 6 CPUs.

Temperature calculated from SVD+LTI ROM. 0.5 hr simulation time with 1 CPU.
Module/Pack Level – Bus Bar Model

Electromagnetic FEA Analysis for Busbar RLC Network Extraction
Module/Pack Level – Bus Bar Model
Voc = -1.031*exp(-35*(abs(IBatt.V/Vinit))) + 3.685 + 0.2156*(abs(IBatt.V/Vinit)) - 0.1178*(abs(IBatt.V/Vinit))^2 + 0.3201*(abs(IBatt.V/Vinit))^3 + 0.3/30.0*(U1.Temp_block_1-273)
Full Battery Simulation
15:00 – Structural Integrity Assessment of a Li-Ion Battery Pack using Simulations. By S. Kottargi, ANSYS India
Conclusions

• Battery is a multi-scale multi-physics application.

• ANSYS provides tools for all aspects of battery simulation.

• Furthermore, ANSYS integrates different models into battery system level simulation through model order reduction.
System Assembly

Embedded Software

- Battery ROM
- Inverter ROM
- Machine ROM
- Behavioral Models

Cruise Control

2013 Automotive Simulation World Congress
October 29 - 30 • Frankfurt am Main, Germany
ROM gives the same results as CFD. ROM runs in less than 5 seconds while the CFD runs 2 hours on one single CPU.


Electrochemistry for Thermal Runaway

- Energy Equation + Heat Source
  - Energy Equation (Default)
    \[ \frac{\partial (\rho c_p T)}{\partial t} = \nabla \cdot \lambda \nabla T + q \]
  - Heat Source (reaction heat + Joule heating)
    \[ q = a_{sj} i_{nj} \left( \phi_s - \phi_e - U_j + T \frac{\partial U_j}{\partial T} \right) \]
    \[ + \sigma_{\text{eff}} \nabla \phi_s \cdot \nabla \phi_s + \left( \kappa_{\text{eff}} \nabla \phi_e \cdot \nabla \phi_e + \kappa_{D} \nabla \ln c_e \cdot \nabla \phi_e \right) \]

Electrochemistry for Thermal Runaway

- Shows impact of material properties on thermal behavior.
- Can also investigate impact of design on thermal behavior, say thickness of the separator.

Numerical Method

• Two user defined scalars are used to solve for $\phi_+$ and $\phi_-$ on CFD mesh.

• $\phi_+$ and $\phi_-$ are loosely coupled through source term, special treatments are used to enhance the convergence for different current, voltage or power boundary condition.

• Sundials IDA solver is used to solve E-chemistry.

• The key is try to reduce the CPU cost!
Cell Level – CFD Thermal

Temperature Distribution
Cell Level – Electro-Thermal

\[ \nabla \cdot (\sigma \nabla \phi) = J \]

\[ J = Y(\phi_c - \phi_a - U) \]
Temperature Distribution - Animation

Temperature calculated from SVD+LTI ROM.
0.5 hr simulation time with 1 CPU.