Computer-Aided Optimization of Macroscopic Design Factors for Lithium-Ion Cell Performance and Life

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Motivation for Battery CAE

Cell/battery development process of testing new materials in multiple cell sizes, in multiple pack designs, and over many months is extremely time consuming, expensive, and ad hoc.

- Large cells/batteries suffer from heat, current, stress issues not present in small configurations

Computer-aided engineering (CAE) processes offer methodology to shorten design cycle and optimize batteries for thermal uniformity, safety, long life, low cost.

- Proven examples from automotive and aerospace
- Robust design, 6-sigma, design optimization,…

Requirements for large battery CAE:
- Efficient mathematical models (desktop PC)
- Capture correct physics and 3D geometry
“Requirements” are usually defined in a macroscale domain and terms

- Wide range of length and time scale physics
- Design improvements required at different scales
- Need for better understanding of interaction among different scale physics
“Requirements” are usually defined in a macroscale domain and terms.
NREL’s Multi-Scale Multi-Dimensional Model Approach
Efficient representation of 3D electrochemical/thermal physics

3D

particle domain dimension

1D

electrode domain dimension

3D

cell domain dimension

10^{-10}  10^{-8}  10^{-6}  10^{-4}  10^{-2}  10^{0} [m]

Design of Materials

Design of Electrode Architecture

Design of Transport at Electrode/Electrolyte

Design of Electron & Heat Transport

Operation & Management

NREL

MSMD-µ  MSMD-c

National Renewable Energy Laboratory

Innovation for Our Energy Future
Importance of Multi-Physics Interaction

Comparison of two 40 Ah flat cell designs
2 min 5C discharge
**Importance of Multi-Physics Interaction**

**Comparison of two 40 Ah flat cell designs**

2 min 5C discharge

- Larger over-potential promotes faster discharge reaction
- Converging current causes higher potential drop along the collectors

**Working potential**

**Electrochemical current production**

**Temperature**
Importance of Multi-Physics Interaction

Comparison of two 40 Ah flat cell designs
2 min 5C discharge

- Larger over-potential promotes faster discharge reaction
- Converging current causes higher potential drop along the collectors
- High temperature promotes faster electrochemical reaction
- Higher localized reaction causes more heat generation
Importance of Multi-Physics Interaction

Comparison of two 40 Ah flat cell designs
2 min 5C discharge

- Larger over-potential promotes faster discharge reaction
- Converging current causes higher potential drop along the collectors
- High temperature promotes faster electrochemical reaction
- Higher localized reaction causes more heat generation

This cell is cycled more uniformly, can therefore use less active material ($) and is expected to have longer life.
Present Study

• Problem definition
  • Model description
  • Macroscopic design parameters chosen for optimization (fixed electrode design)
  • Design evaluation criteria
  • Optimization procedure (numerical DoE)

• Results
  • Response surface
  • Optimal designs

• Conclusions
Model Realization for 20 Ah Stacked Prismatic Cell

- Reduced order model derived from governing equations of Doyle, Fuller, Newman, 1993.
- Chose parameters representative of NCA/graphite chemistry.
- Stacked prismatic design
- Various form factors
- Tabs on same side
- 20 Ah
- PHEV10 application

**1D**

- Particle domain dimension

**1D**

- Electrode domain dimension

**2D**

- Cell domain dimension

- SVM

- 15 mm

- 10 mm-50 mm
Macroscopic Design Parameters Chosen for Optimization

Aspect ratio, $H/W$
Tab width, $\theta/W$
Electrode layers, $N$
Foil thickness, $\delta_{Cu}$

Other design parameters fixed:
- $\delta_{Al} = 1.6 \times \delta_{Cu}$
- 20 Ah capacity
- Electrode loadings
- Electrode thicknesses

(Typical tradeoff between power & energy do not arise in this study)
Cell Design Evaluation Criteria

Energy at 2C rate

- Energy density (Wh/L) evaluated at module level (includes 5mm external tab height + 3 mm cooling channel between cells)

Maximum temperature during driving cycle

- 10-mile PHEV charge depletion cycle

Baseline design

71 Wh

51°C peak
Optimization Process Steps - 1

1. Use Design Of Experiments to generate 50 design points
2. Execute NREL’s 3D Electrochemical-Thermal Multi-Physics Model for all 50 DOE points
3. From the 50 DOE points use an advanced response surface technique (Radial based Functions) to generate 4 response surface functions:
   a) $T_{max} (N_{layers}, t_{CU}, H_W, t_{Tab}_W)$
   b) Energy_Density ($N_{layers}, t_{CU}, H_W, t_{Tab}_W$)
   c) Specific_Energy ($N_{layers}, t_{CU}, H_W, t_{Tab}_W$)
   d) Cell Thickness ($N_{layers}, t_{CU}, H_W, t_{Tab}_W$)

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4. Generate 1000 more DOE points using a simple sampling technique (Sobol)

5. Run the 1000 DOE points through the 4 response functions to generate 1000 more data points

6. Select the best of the 1050 design points and use it as starting point for an optimization algorithm

7. The optimizer tries to maximize the energy density with two constraints a) $T_{\text{max}} < 55 \, \text{C}$ and b) $L < 16 \, \text{mm}$

8. Identify the top two optimum points
More layers reduces Tmax by creating shorter, parallel paths for e⁻ flow

Thicker foil reduces ohmic losses

Thinner foil shortens thermal diffusion length

Minimum Tmax
Energy Density* versus Number of Layers & Cu Foil Thickness

More parallel layers reduces losses, maximizes useable energy

Less foil reduces volume, mass of inert components

*2C rate, module level Wh/L
Increasing tab width (larger circles) reduces excessive current convergence near terminals, reduces Tmax.
Scatter Plot of Tmax versus Energy Density
Feasible points with Tmax < 55°C
Scatter Plot of Tmax versus Energy Density
Feasible points with Tmax < 55°C and Cell thickness < 16 mm
Effect of Design Variables on $T_{\text{max}}$ (minimize)

- Increase number of layers (up to some limit)
- Increase tab width
- Increase cell height
- Decrease foil thickness

Design Factors:
- $N_{\text{layers}}$
- $t_{\text{Tab}\_W}$
- $H\_W$
- $t_{\text{CU}}$

Effect Size – $T_{\text{max}}$ (°C)
Optimum Design

Point #1

Optimum Design

Point #2
## Optimal vs. Base Cell Design

### Design Parameters Simulated Performance

<table>
<thead>
<tr>
<th></th>
<th>N Layers</th>
<th>Cu foil thickness</th>
<th>H (mm)</th>
<th>L (mm)</th>
<th>Energy Density* (Wh/L)</th>
<th>US06 Tmax (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>19</td>
<td>10</td>
<td>248</td>
<td>6.3</td>
<td>166</td>
<td>50.6</td>
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<td>Opt1</td>
<td>36</td>
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<td>187</td>
<td>16.2</td>
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<tr>
<td>Opt2</td>
<td>32</td>
<td>12.3</td>
<td>191</td>
<td>16.6</td>
<td>261</td>
<td>39.5</td>
</tr>
</tbody>
</table>

*module level energy density includes 5mm external tab height & fixed 3mm intercell gap

- More layers
- Shorter height
- Improved energy density
- Peak temperatures reduced 10°C
Conclusions

- Large cell design is a challenging problem of competing requirements & objectives.
- Robust design CAE methods provide a straightforward process for optimization, so long as:
  - Objectives & constraints are well-defined.
  - Physics and geometry are properly captured.
- Compared to baseline design, optimization of macroscopic factors decreases peak temperatures (fewer losses in cell) while increasing useable energy density.
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