Evaluation Study for Large Prismatic Lithium-Ion Cell Designs Using Multi-Scale Multi-Dimensional Battery Model

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Batteries for Electrified Vehicles

Electrified drive-train vehicles such as PHEVs and EVs with range-extenders are believed to be near-term technologies that are
- displacing significant petroleum use in the transportation sector
- diversifying energy sources for mobility

Advances in batteries are critical to realize green mobility technologies

DOE’s Energy Storage System Performance Targets for PHEVs

<table>
<thead>
<tr>
<th>Characteristic of Use (End-of-Life)</th>
<th>Minimum PHEV Battery</th>
<th>Maximum PHEV Battery</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference Equivalent Electric Range</td>
<td>10 miles</td>
<td>40 miles</td>
</tr>
<tr>
<td>Peak Discharge Power (C sec 10 sec)</td>
<td>kW</td>
<td>240-348</td>
</tr>
<tr>
<td>Peak Repeat Pulse Power (10 sec)</td>
<td>kW</td>
<td>20-25</td>
</tr>
<tr>
<td>Max. Current (10 sec pulse)</td>
<td>A</td>
<td>140-160</td>
</tr>
<tr>
<td>Available Energy for CD Charge-Dephasing Mode, 10 kW Race</td>
<td>kWh</td>
<td>3.4-11.6</td>
</tr>
<tr>
<td>Available Energy for CD Charge-Sustaining Mode, 10 kW Rate</td>
<td>kWh</td>
<td>0.6-3.3</td>
</tr>
<tr>
<td>Minimum Round trip Energy Efficiency (CS 50 Wh profile)</td>
<td>%</td>
<td>50-60</td>
</tr>
<tr>
<td>Cold cranking power at -30°C, 2 sec, 3 Peaks</td>
<td>kW</td>
<td>5-7</td>
</tr>
<tr>
<td>CD Life/Discharge Throughtput</td>
<td>Cycles/MWh</td>
<td>5,000 / 17</td>
</tr>
<tr>
<td>CS HV Cycle Life 50 Wh Pulse</td>
<td>Cycles</td>
<td>100,000</td>
</tr>
<tr>
<td>Calendar Life, 57°C</td>
<td>Year</td>
<td>9 - 11</td>
</tr>
<tr>
<td>Maximum System Weight</td>
<td>kg</td>
<td>60-120</td>
</tr>
<tr>
<td>Maximum System Volume</td>
<td>Liter</td>
<td>40-80</td>
</tr>
<tr>
<td>Maximum Operating Voltage</td>
<td>Vdc</td>
<td>480-640</td>
</tr>
<tr>
<td>Maximum Operating Voltage</td>
<td>Vdc</td>
<td>480-640</td>
</tr>
<tr>
<td>Maximum Self-discharge</td>
<td>Wh/kg</td>
<td>10-50</td>
</tr>
<tr>
<td>Maximum System Recharge Rate at 30°C</td>
<td>kW</td>
<td>1.4 (120V/150A)</td>
</tr>
<tr>
<td>Unusual Operating &amp; Charging Temperature Range</td>
<td>°C</td>
<td>-30 to +65</td>
</tr>
<tr>
<td>Survival Temperature Range</td>
<td>°C</td>
<td>-65 to +166</td>
</tr>
<tr>
<td>Maximum System Production Price</td>
<td>$/100 Wh units</td>
<td>$1,700-5,000</td>
</tr>
</tbody>
</table>

Table 1. Energy Storage System Performance Targets for Plug-In Hybrid Electric Vehicles (January 2007)
Batteries for Electrified Vehicles

Electrified drive-train vehicles such as PHEVs and EVs with range-extenders are believed to be near-term technologies that are
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### DOE’s Energy Storage System Performance Targets for PHEVs

<table>
<thead>
<tr>
<th>Characteristics at EOL (End-of-Life)</th>
<th>Unit</th>
<th>Minimum PHEV Battery</th>
<th>Maximum PHEV Battery</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference Equivalent Electric Range</td>
<td>miles</td>
<td>10</td>
<td>40</td>
</tr>
<tr>
<td></td>
<td>Peak Regen Pulse Power (10°/s)</td>
<td>kW</td>
<td>20</td>
</tr>
<tr>
<td></td>
<td>Max Current (10 sec pulse)</td>
<td>A</td>
<td>100</td>
</tr>
<tr>
<td>Available Energy for CD (Charge-Depleting) Mode, 10-kW Rate</td>
<td>kWh</td>
<td>3.4</td>
<td>11.6</td>
</tr>
<tr>
<td></td>
<td>Cold cranking power at -30°C, 5 sec, 3</td>
<td>kW</td>
<td>2</td>
</tr>
<tr>
<td>Maximum System Weight</td>
<td>kg</td>
<td>60</td>
<td>120</td>
</tr>
<tr>
<td>Maximum System Volume</td>
<td>Liter</td>
<td>40</td>
<td>80</td>
</tr>
<tr>
<td>CD Life / Discharge Throughput</td>
<td>Cycles/MWh</td>
<td>5,000 / 17</td>
<td>5,000 / 58</td>
</tr>
<tr>
<td>CS HEV Cycle Life, 50 Wh Profile</td>
<td>Cycles</td>
<td>300,000</td>
<td>300,000</td>
</tr>
<tr>
<td>Calendar Life, 35°C</td>
<td>year</td>
<td>15</td>
<td>15</td>
</tr>
<tr>
<td>Maximum System Production Price @ 100k units/yr</td>
<td>$</td>
<td>$1,700</td>
<td>$3,400</td>
</tr>
</tbody>
</table>
Multi-Scale Physics in Li-Ion Battery

Requirements & Resolutions

“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
Multi-Physics Interaction

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

working potential

working potential

electrochemical current production

electrochemical current production

temperature

temperature
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
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

Electrochemical current production

- 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 has longer life.
Electrode-Scale Performance Model

Charge Transfer Kinetics at Reaction Sites

\[ j^{Li} = a_s i_o \left( \exp \left[ \frac{\alpha_a F}{RT} \eta \right] - \exp \left[ -\frac{\alpha_c F}{RT} \eta \right] \right) \]

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

Species Conservation

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

\[ \frac{\partial (\epsilon c_e)}{\partial t} = \nabla \cdot (D_e^{\text{eff}} \nabla \epsilon) + \frac{1 - t^o}{F} j^{Li} - \frac{i_e \nabla t^o}{F} \]

Charge Conservation

\[ \nabla \cdot (\sigma^{\text{eff}} \nabla \phi_e) - j^{Li} = 0 \]

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

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 group (Doyle, Fuller, and Newman 1993)
- Captures lithium diffusion dynamics and charge transfer kinetics
- 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
To expand knowledge of the impacts of *designs in different scales*, usages, and management on performance, life, and safety of battery systems.

*Simply* Work?

*Extend model domain size up to cell scale to capture macroscopic design features, while maintaining model resolution to capture Li diffusion dynamics in electrode level scale* ??? → huge computational complexity and cost
Approach

Multi-Scale Multi-Dimensional (MSMD) Model

- Captures macroscopic electron/heat transports, electrode scale Li diffusion dynamics/charge transfer kinetics in separate domains
- Physically couple the solution variables defined in each domain using multi-scale modeling schemes
- Runs in tolerable calculation time, practical for battery and system engineering design
"Poorly designed electron and heat transport paths can cause excessive spatial non-uniformity in battery physics, and then deteriorate the performance and shorten the life of the battery."

**Objectives**
Demonstrate the impact of macroscopic design factors on battery …
- **Performance**: B2 abs# 252 (Kim & Smith) ➔ This talk
- **Life**: B2 abs# 255 (Smith & Kim)
Nominal Design – 10C discharge for 30 sec

- Stacked prismatic design
- 140 x 100 x 15 mm³ form factor
- Tabs on a same side
- 20 Ah
- PHEV10 application

- 10C constant current discharge
- soc ini = 90%
- Surface and tab cooling
- h inf = 20 W/m²K
- Tamb = 30°C
- Tin = 30°C

V(t)
OCV(t)
evaluated from volumetric average of composition
Electrical Response – 10C Discharge

Current density field at metal collector foils after 30 sec discharge at mid-plane

Working potential between electrode planes after 30 sec discharge at mid-plane

Al foil

Cu foil
Electrical Response – 10C Discharge

Current density field at metal collector foils after 30 sec discharge at mid-plane

Working potential between electrode planes after 30 sec discharge at mid-plane

Large Overpotential
Thermal Response – 10C Discharge

Temperatures after 30 sec discharge

- $T_{ini} = 30.0 \, ^{\circ}C$
- $T_{avg} = 34.3 \, ^{\circ}C$
- $\Delta T = 2.3 \, ^{\circ}C$

Tini = 30.0 $^\circ$C
Tavg = 34.3 $^\circ$C
$\Delta$T = 2.3 $^\circ$C
Electrochemical Response – 10C discharge

Discharge current density

SOC- \( \text{SOC}_{\text{avg}} \)

\[
\text{soc}(t) \quad [\%]
\]

\[
t \quad [\text{s}]
\]

average soc
maximum soc
minimum soc
Virtual Design Evaluation

Virtual Battery Design

Vehicle Design

Embedded Battery Model

Vehicle Simulator

Multi-Scale Multi-Dimensional Li-ion Battery Model

Vehicle Driving Profile

Battery Power Profile

Battery Responses

Feedback

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Alternative Cell Designs

**Nominal Design**
- 140 x 100 x 15 mm\(^3\)
- Tabs on a same side
- 20 Ah

**Small Capacity (SC)**
- 3 x (140 x 100 x 5) mm\(^3\)
- Same tab design
- 3 x 6.67 Ah
- Same electrode area/stack layer
- 1/3 thickness
- ~3x surface area

**Thin and Wide (TW)**
- 200 x 140 x 7.5 mm\(^3\)
- Same tabs
- 20 Ah
- 2x electrode area/stack layer
- 1/2 thickness
- ~2x surface area

**Counter Tab (CT)**
- 250 x 120 x 7 mm\(^3\)
- Wide-counter tab design
- 20 Ah
- ~2x electrode area/stack layer
- ~1/2 thickness
- ~2x surface area
Thermal Behavior Comparison

Battery Power Profile

mid-size sedan PHEV10 US06 drive

- 15-minute drive (CD + CS)
- $\text{soc}_{\text{ini}} = 90\%$
- Surface and tab cooling
- $h_{\text{inf}} = 20 \text{ W/m}^2\text{K}$
- $T_{\text{amb}} = 30^\circ\text{C}$
- $T_{\text{ini}} = 30^\circ\text{C}$
Temperature Imbalance during CD Drive

@ $t = 6$ min

Nominal

TW

CT

SC

@ $t = 6$ min

T_{avg}(t) [°C]

$\Delta T(t)$ [°C]

t [min]
Temperature Imbalance during CS drive

@ t=15 min

Nominal

TW

CT

SC

Nominal

@ t=15 min

SC

CT

TW

0 5 10 15 t [min]

36 38 40 42 44 46 48

0 5 10 15 t [min]

25 30 35 40 45 50 55

T_{avg}(t) [°C]

ΔT(t) [°C]

$T_{avg}(t)$ [°C]

$ΔT(t)$ [°C]

$T_{avg}(t)$ [°C]

$ΔT(t)$ [°C]
Ah Throughput Imbalance $TW$ vs $CT$

Ah/m$^2$

$V_{oc}$ [V]

t [min]

$V_{oc}$ vs $t$

Ah Throughput Imbalance

Ah/m$^2$ vs $XY$

$TW$ vs $CT$

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Summary

- **Nonuniform battery physics**, which is more probable in large-format cells, can cause unexpected performance and life degradations in lithium-ion batteries.
- A **Multi-Scale Multi-Dimensional model** was used for evaluating large format prismatic automotive cell designs by integrating micro-scale electrochemical process and macro-scale transports.
- **Thin form factor prismatic cell with wide counter tab design** would be preferable to manage cell internal heat and electron current transport, and consequently to achieve uniform electrochemical kinetics over a system.

Engineering questions to be addressed in further discussion include …
- **What is the optimum form-factor and size of a cell?**
- **Where are good locations for tabs or current collectors?**
- **How different are externally proved temperature and electric signals from non-measurable cell internal values?**
- **Where is the effective place for cooling? What should the heat-rejection rate be?**
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