Multi-Scale Multi-Dimensional Model
for Better Cell Design and Management

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"Requirements" are usually defined in a macroscale domain and terms.
Need a Multi-Scale Model?

Numerical approaches focusing on different length scale physics

a) Quantum mechanical and molecular dynamic modeling
b) Numerical modeling for addressing the impacts of architecture of electrode materials
c) 1D performance model capturing solid-state and electrolyte diffusion dynamics
d) Cell-dimension 3D model for evaluating macroscopic design factors
Why macro-scale transport becomes critical?

Sub-electrode scale physics
Kinetics
Li diffusion
Ion transport
Heat dissipation

Design of current and heat flow paths

Spatial variation of ...
• Electric potentials
• Temperatures

Size Effect

Flux (gradient)  
Barrier (distance)

Spatial Difference (gradient x distance)
Approach in the Present Study

**Multi-Scale Multi-Dimensional (MSMD) Modeling**

*To address ...*
- Multi-scale physics from sub-micro-scale to battery-dimension-scales
- Difficulties in resolving microlayer structures in a computational grid

Simulation Domain = Macro Grid + Micro Grid

*Image source: www.dimec.unisa.it*
Solution Variables

NOTE:
Selection of solution scheme for either grid system is independent of the other.
Previous Study

AABC 08, Tampa, May 2008

"Poorly designed electron and heat transport paths can cause excessive nonuniform use of materials and then deteriorate the performance and shorten the life of the battery."
Analysis

Comparison with Experimental Results

- Model Validation against JCS VL41M Test Data

Macro-Scale Design Evaluation Analysis

- Impacts of Aspect Ratio of a Cylindrical Cell
Comparison with Experimental Results

Model Validation against JCS VL41M Test Data

The JCS VL41M cell was chosen as a candidate for several reasons:
- 1-D electrochemical model was previously validated vs. VL41M current/voltage data.
- Thermal imaging experiments were recently run.
- Future calorimeter test data will allow for further refinement & validation of the model.

Macro-Scale Design Evaluation Analysis

Impacts of Aspect Ratio of a Cylindrical Cell
Approach

1) 1-D Electrochemical Model Validation
   - Measured current & temperature profiles used as inputs to model
   - Model predicts voltage & heat generation rate

2) Multi-Scale Multi-Dimensional (“MSMD”) Model Validation
   - Utilized 3D thermal model results to extract thermal boundary conditions
   - Measured surface temperature compared to model prediction of jelly-roll surface temperature.

3) MSMD Model Predictions
   - Multidimensional features
1) 1D Electrochemical Model Validation

Measured current and skin temperature profiles from thermal imaging test used as inputs to lumped thermal/1-D electrochemical model.

Model voltage prediction compares favorably with data.
- Error generally < 50 mV

Test Profile:
5 charge-depletion cycles + 60 charge-sustaining cycles per USABC manual (BSF = 39)

* Skin temperature measured via thermocouple on can wall, 3" from bottom.
1) 1D Electrochemical Model Validation

Test Profile:
5 charge depletion cycles + 60 charge sustaining cycles per USABC manual (BSF = 39)

Irreversible heat generation rate predicted by 1-D electrochemical model compares well with calculated value using measured current and voltage and model open-circuit voltage.

\[ Q_{\text{irr}} = I_{\text{meas}} (OCP_{\text{model}} - V_{\text{meas}}) \]

- Entropic heat effects seem to be non-negligible and may need to be included in the model.

* More rigorous heating rates and specific heat to be measured in upcoming calorimeter testing.
2) MSMD Model Validation

Assumption for Model Simplification

Note: The schematics shown above do not represent actual JCS VL41M.
2) MSMD Model Validation

Retrieving information from 3D Thermal Model for MSMD model input

- Complex thermal pathway was captured in 3D thermal model, then appropriate thermal boundary condition was evaluated for MSMD model.

- General system response for temperature distributions at cell skins, terminals and bus bars is well predicted and reveals how heat is transferred through the 3 cell assembly.
2) MSMD Model Validation

**Evaluating thermal boundary conditions at jelly-roll surfaces**

**Area Weighted Averages**

- \( h_{\text{top}} = 22.6 \, \text{W/m}^2\text{K} \)
- \( h_{\text{side}} = 8.7 \, \text{W/m}^2\text{K} \)
- \( h_{\text{bottom}} = 12.4 \, \text{W/m}^2\text{K} \)

**Heat transfer coefficient at jelly-roll surfaces of the middle cell**

\( h_{\text{inf}} = 8 \, \text{W/m}^2\text{K} \)
2) MSMD Model Validation

Comparison with Measured Temperature

Measured can surface temperature and model-predicted jelly-roll temperature agree reasonably well. Without an internally-instrumented cell, it is not possible to directly validate the MSMD model’s jelly-roll temperature predictions.
3) MSMD Model Prediction

Snapshots at the end of CHARGE DEPLETING cycles

- \( t = 1770 \) s
- \( T_{\text{can wall}} = 31.6^\circ\text{C} \)
- Current = 409 A

Heat Transport

Temperature

- \( \text{max}(T) - \text{min}(T) = 1.4^\circ\text{C} \)

Potential

- Electron Transport

Potential

- Positive end
- Negative end

Reaction Current

- \( \frac{\text{max}(I) - \text{min}(I)}{\text{avg}(I)} = 1.6\% \)

SOC

- \( \text{max}(\text{SOC}) - \text{min}(\text{SOC}) = 0.24\% \)
3) MSMD Model Prediction

**Ah-throughput during CHARGE DEPLETING cycles**

- $t = 1770 \text{ s}$
- $T_{\text{can wall}} = 31.6^\circ \text{C}$
- Current = 409 A

**Temperature at the end of CD cycles**

**Ah-throughput imbalance during CD cycling**

$\frac{(\text{Ah/m}^2 - \text{Ah/m}^2_{\text{avg}})}{\text{Ah/m}^2_{\text{avg}}}$
Analysis

Comparison with Experimental Results

Model Validation against JCS VL41M Test Data

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Macro-Scale Design Evaluation Analysis

Impacts of Aspect Ratio of a Cylindrical Cell
Aspect Ratio of Cylindrical Cells

PHEV10 application
- US06 cycle discharges 3.4 kWh in 12 minutes (~3C rate)

20 Ah cell
- Well suited for PHEV10
- BSF = 78 → $V_{nom} \approx 290V$

US06 CD cycle
- $P_{avg} = 14$ kW, $P_{RMS} = 32$ kW
Brief Look at “What H/D Ratio Means”

Volume = const

H x W = const

Foil thicknesses
Al: 20 µm
Cu: 15 µm

\[ P_{\text{loss, foil}} \sim \frac{\rho \cdot i'^2}{\delta} H^2 \]

\[ \Delta V_{\text{foil}} \sim \frac{\rho \cdot i''}{\delta} H^2 \]

\( i'\): current [A/m²]
\( \rho \): resistivity
\( \delta \): foil thickness
10s Power Capability Comparison

**Large H**
- D[mm]: 28
- H[mm]: 350

**Nominal**
- D[mm]: 50
- H[mm]: 107

**Large D**
- D[mm]: 115
- H[mm]: 20

- Large H design has almost 10% less power capability.

![Graph showing power capability comparison](image)
US06 CD Cycle x 2, Natural Convection

Large H cell has greatest temperature rise owing to long electronic current paths resulting in high foil heating.

Foil heat contribution to total:
- 15% - Large H
- 1.7% - Nominal
- <0.1% - Large D

Large H cell has greatest internal temperature imbalance.
US06 CD Cycle x 2, Natural Convection

Amp-hour Throughput Imbalance

- Large Dia. Cell: -0.1% to +0.03%
- Nominal Cell: -0.2% to +0.3%
- Large Height Cell: -1.2% to +2.9%

\[
\frac{(Ah/m^2 - Ah/m^2_{avg})}{Ah/m^2_{avg}}
\]
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 developed as a tool for investigating interaction between micro-scale electrochemical process and macro-scale transports using a multi-scale modeling scheme.

- The developed model will be used to provide better understanding and help answer **engineering questions** about improving **cell design**, **cell operational strategy**, **cell management**, and **cell safety**.

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- Engineering questions to be addressed in **future works** include …

  - What is the optimum form-factor and size of a cell?
  - Where are good locations for tabs or current collectors?
  - How different are measured parameters from their nonmeasurable internal values?
  - Where is the effective place for cooling? What should the heat-rejection rate be?
  - How does the design of thermal and electrical paths impact under current-related safety events, such as internal/external short and overcharge?
Acknowledgments

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• Ahmad Pesaran
Thank you!
Additional Slides
- Skin temperature of Cell C is low, because it is directly connected to the cable through the positive terminal.
- There are inflows of heat through the positive thermals at Cell A and Cell B which are connected to the negative terminals of the neighbor cells.
- Most heat is rejected through cell side surfaces. About 10% of heat is dissipated at bus bar surfaces. 12% runs away through cables.
3) MSMD Model Prediction

**Temperature Distribution after 30 sec 300 A discharge**

**Temperature Distribution after 20 min 100 A geometric cycling**
US06 CD Cycle x 2, Natural Convection

Temperature Distribution

Tmax - Tmin = 1.7°C
Tavg = 44.7°C

Tmax - Tmin = 1.7°C
Tavg = 45.5°C

Tmax - Tmin = 3.2°C
Tavg = 47.6°C
US06 CD Cycle, Natural Convection

Integrated Heat Imbalance

Large Dia. Cell
-0.1% to +0.1%

Nominal Cell
-1.1% to +2.7%

Large Height Cell
-9% to +21%

US06 CD cycle
Forced Convection

Natural Convection  
(h = 8 W/m² K)

Forced Air Convection  
(h = 30 W/m² K)

Average temperature lower

~ 5°C in Large H and Large D format, ~2°C in Nominal

Heat generation similar

Temperature imbalance 1-3°C higher
Forced convection – negligible impact on where heat is generated

Integrated Heat Imbalance

**Large Dia. Cell**
Natural: -0.1% to +0.1%
Forced: -0.3% to +0.2%

**Nominal Cell**
Natural: -1.1% to +2.7%
Forced: -1.2% to 2.8%

**Large Height Cell**
Natural: -9% to +21%
Forced: -9% to +21%

US06 CD cycle
Despite additional thermal imbalance, forced convection does not drastically change localized material usage.

### Amp-hour Throughput Imbalance

**Large Dia. Cell**
- Natural: -0.1% to +0.03%
- Forced: -0.3% to 0.07%

**Nominal Cell**
- Natural: -0.2% to +0.3%
- Forced: -0.3% to 0.4%

**Large Height Cell**
- Natural: -1.2% to +2.9%
- Forced: -1.3% to 2.9%

*US06 CD cycle*
Comparison of natural and forced convection

at $t = 690$ s of US06 cycle

<table>
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<th>$T_{avg}$ (°C)</th>
<th>$T_{max} - T_{min}$ (°C)</th>
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