Coupled Mechanical-Electrochemical-Thermal Modeling for Accelerated Design of EV Batteries

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Introduction

I. The physical phenomena occurring in a battery are many and complex and, in different scales (particle, electrodes, cell, pack)
   1. Electrochemical (e.g., node-cathode interactions)
   2. Electrical (e.g., electron moving in the current collectors)
   3. Thermal (e.g., heat release due cell inefficiencies)
   4. Chemical (e.g., electrolyte reactions with electrode surfaces)
   5. Mechanical (e.g., pressure build-up, deformation after a crush)

II. Better understanding of interplay between different physics occurring in different scales through modeling could provide insight to design improved batteries for electric vehicles

III. Work funded by U.S. DOE has resulted in development of computer-aided engineering (CAE) tools to accelerate electrochemical and thermal design of batteries; mechanical modeling is underway

IV. This paper provides an overview of the M-ECT modeling efforts
Battery Modeling at NREL

NREL has developed a unique set of multi-physics, multi-scale modeling tools for simulating performance, life, and safety of lithium-ion batteries.
**Li-Ion ECT Modeling: Porous Electrode Theory**

**Charge Transfer Kinetics at Reaction Sites**

\[ j_{Li} = \alpha_a i_e \left\{ \exp \left[ \frac{\alpha_a F}{RT} \eta \right] - \exp \left[ -\frac{\alpha_e F}{RT} \eta \right] \right\} \]

\[ i_0 = k (c_e)^{\alpha_a} (c_{s,\text{max}} - c_{s,e})^{\alpha_a} (c_{s,e})^{\alpha_e} \]

**Species Conservation**

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

\[ \frac{\partial (\varepsilon_e \rho_e)}{\partial t} = \nabla \cdot \left( \sigma_{\text{eff}} \nabla \phi_s \right) + \frac{1-f_e^2}{F} j_{Li} - \frac{i_e}{F} \nabla f_e \]

**Charge Conservation**

\[ \nabla \cdot \left( \sigma_{\text{eff}} \nabla \phi_s \right) - j_{Li} = 0 \]

\[ \nabla \cdot \left( \Lambda_{\text{eff}} \nabla \phi_s \right) + \nabla \cdot \left( \Lambda_{\text{D}} \nabla \ln c_e \right) + j_{Li} = 0 \]

**Energy Conservation**

\[ \frac{\partial e}{\partial t} + \nabla \cdot (k \nabla T) + q = \frac{\partial e}{\partial t} + \nabla \cdot (k \nabla T) + q = \]

- Pioneered by John Newman group at University of California–Berkeley (*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 apply in large format batteries where *heat* and *electron current* transport critically affect the battery responses
NREL’s MSMD Li-Ion Modeling Framework

Through the multi-year effort supported by U.S. DOE, NREL has developed a modeling framework for predictive computer simulation of Li-ion batteries known as the **Multi-Scale Multi-Domain (MSMD)** model, which addresses the interplay among the physics in varied scales and extends the porous electrode modeling:

The model quantifies the impacts of the electrical/thermal pathway design on uneven charge-discharge kinetics in large format wound prismatic cells.
Understanding Non-Uniform Utilization

Developing CAE Battery Modeling Tools

I. Realizing the need to develop CAE tools, U.S. DOE initiated the CAEBAT project in 2010

II. Partnerships between national labs, battery developers, software providers, universities, and carmakers were established

III. With technical support from NREL and Oak Ridge National Laboratory, three independent teams developed competitive CAE battery tools

IV. CAEBAT tools are now available for purchase
   1. EC Power’s battery design software is called AutoLion™
   2. CD-adapco’s battery simulation module is available in STAR-CCM+
   3. ANSYS’s battery design tools are an integral part of Fluent 15 and 16
CAEBAT Tools for Battery Design

CAEBAT tools could:
I. Predict electrochemical, electrical, and thermal performance of a cell based on geometry, chemistry, and power load
II. Simulate performance of a battery pack with various thermal management designs
III. Provide insight on the safety and life implications of different loads and designs
Battery Crush and Thermal Runaway

Going beyond today’s approach: Battery as a brick

Li battery safety a major concern – need to have CAE tools
Battery crush $\rightarrow$ damaged zone $\rightarrow$ failure of separator
Electrode contacts $\rightarrow$ local short $\rightarrow$ current flow $\rightarrow$ heat generation
Heat generation without rejection $\rightarrow$ temperature increase
Reaching above onset temperature $\rightarrow$ spontaneous reactions $\rightarrow$ thermal runaway $\rightarrow$ smoke and fire

$: may lead to depending on many factors
Modeling Battery Mechanical Crush

I. Electric vehicles (EVs) must be as safe as other road vehicles, particularly during a crash; need to understand crushed battery’s thermal response

II. In 2014, U.S. DOE initiated the 2nd phase of CAEBAT to include modeling mechanical behavior during EV crash-induced crush

III. NREL initiated collaborating with others to develop coupled mechanical-electrochemical-thermal models to predict the response of cells or modules upon structural failure

1. Simulating simultaneous mechanical, electrochemical, and thermal response of a cell or module due to crush is very complex and requires modeling simplifications

2. Crush is an event that usually happens in less than 1/10th a second while subsequent electrochemical and thermal responses take much longer

3. Our approach is to model structural behavior first; capture the characteristics of damaged zone and use it for electrochemical and thermal modeling to see if thermal runaway could occur

4. This allows us to link the mechanical aspect with the thermal aspect in a sequential, one-way fashion
I. Crashworthiness lab at MIT performing multi-axial strain measurements

II. Digital Image Correlation used to reduce measurements to material properties for input into LS-DYNA

III. These models are used to predict origin of cracks
Progress to Date: Cell Crush Modeling

To obtain the structural deformation of layers of cell upon a specified crush and to predict short circuit, we need a refined model to represent each individual layer of current collector, anode, cathode, and separator.

Through-thickness architecture
Multiple layers in a cell

Simplified representative sandwich (RS) with equivalent mechanical properties

<table>
<thead>
<tr>
<th>Choice of Model</th>
<th>Total # of layers</th>
</tr>
</thead>
<tbody>
<tr>
<td>RS model</td>
<td>8</td>
</tr>
<tr>
<td>Full model</td>
<td>166</td>
</tr>
</tbody>
</table>

MIT experiment
Single RS model simulation
Full battery model simulation
**Compression**

Top rigid wall moves down quasi-statically

Bottom rigid walls fixed

A small friction coefficient (0.01) is defined between the rigid wall and battery to avoid numerical instability.

**Indentation**

Rigid sphere wall moves down quasi-statically

In the present work, fracture (material failure, element deletion) is not considered.

The RS model can correlate with the whole battery model. It can be used to study the individual deformation mechanism and structure-electric-thermal coupled responses.
Mechanical Simulation: Individual Deformation

1. Indentation-induced damage is more localized and complicated
2. Separator is very likely the first to fail
Mechanical-Thermal-Electric Coupled Simulation: LS-DYNA Multi-physics Solver

Studies on conducted to predict the electro-thermal responses. As preliminary investigation, only the single RS model is studied.

• Sequential mechanical-electric-thermal coupled analysis:
  • The RS model is first analyzed using LS-DYNA Explicit
  • The deformed shape at a certain stage is exported into a independent mesh file
  • Electro-thermal model is then built on the deformed mesh and solved using LS-DYNA multi-physics solver (can be done in ANSYS/Fluent)
I. Simplified method to couple mechanical crush with the electrical response of the cell that has computational time of a few minutes.

II. Our approach uses multiple criteria to evaluate short-circuit under deformation:
- mechanical failure of components
- drop in electrical resistance across the short-circuit
- temperature-based failure criterion

An adiabatic (perfectly insulated) thermal boundary condition is used.

\[ T_{\text{max}} = 398^\circ \text{C} \]
Linking Deformed Geometry in a Cell to Electrochemical-Thermal Models in CAEBAT
Proposed Approach for Linking Mechanical to ECT - 1

Initial Geometry

Crush Simulations in LS-DYNA

Export Deformed Mesh to ANSYS

Compute Individual Resistances

Perform ECT Simulations

The benefit of using this approach of existing electrochemical-thermal (ECT) in ANSYS/Fluent developed under CAEBAT phase 1

C. Yang et al., 225th ECS Meeting, May 2014, Orlando, FL
Proposed Approach for Linking Mechanical to ECT - 2

**Initial Geometry**

**Crush Simulations in LS-DYNA**

**Export Deformed Mesh to ANSYS**

**Compute Individual Resistances**

**Perform ECT Simulations**

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**Advantage:**
- Better integration of electrical simulations with ECT

**Challenges:**
- Performing ECT simulations on the deformed mesh
- Simultaneously solving for resistance distribution and current distribution in Fluent: implications on short-circuit simulations using ECT

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Summary

I. Electrochemical-thermal tools under CAEBAT-1
   1. U.S. DOE initiated the development of battery CAE tools for battery design
   2. Three competitive CAE tools are now commercially available

II. Coupling ETC models with mechanical models for simulating cell under indentation and compression (CAEBAT-2)
   1. Incorporating all cell layers, a refined representative sandwich (RS) model is built
   2. The RS model is able to capture the global stress-strain response and predict the local deformation of each component
   3. At the sub-cell level, an anisotropic constitutive model was developed and calibrated against experiments
   4. We also have developed a methodology to capture evolution of contact area during the short circuit
   5. Sequential coupled structure-electric-thermal simulations were conducted using the RS model, which produced reasonable electrical and thermal responses
Future Work – Mechanical ECT Modeling

I. Obtain mechanical properties of various cells and electrodes

II. Further refine the finite element model and apply it to pouch cells with the packaging material

III. Implement fracture in the mechanical simulation

IV. Develop criteria for short circuit using the developed mechanical-electrical-thermal model

V. Sequential analysis using the ANSYS ECT model

VI. Perform simulations of mechanical ECT for a typical crash-induced crush for a cell

VII. Perform experiments on crushing a cell to thermal runaway

VIII. Compare experimental data with the simulation results for refining the model
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