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, 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 \textit{modeling} will provide insight to designing improved batteries for electric vehicles

III. Work funded by US DOE has resulted in development of computer aided engineering tools to accelerate electrochemical and thermal design of batteries; mechanical modeling 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**

\[
j_{Li}^{1} = a_z i_o \left( \exp \left( \frac{\alpha_{z,F}}{R T} \right) - \exp \left( - \frac{\alpha_{c,F}}{R T} \right) \right)
\]

\[
i_o = k(c_e)^{\alpha_a} (c_{z,max} - c_{z,e})^{\alpha_z} (c_{z,e})^{\alpha_c} \eta = (\phi_z - \phi_e) - U
\]

**Species Conservation**

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

\[
\frac{\partial (c_z c_e)}{\partial t} = \nabla \cdot \left( D_{eff} \nabla c_e \right) + \frac{1 - r^o}{F} j_{Li}^{1} - \frac{1}{F} \nabla \cdot \nabla I^{o}
\]

**Charge Conservation**

\[
\nabla \cdot (\sigma_{eff} \nabla \phi_{e}) - j_{Li}^{1} = 0
\]

\[
\nabla \cdot (\kappa_{eff} \nabla \phi_{s}) + \nabla \cdot (\kappa_{D}^{eff} \nabla \ln c_s) + j_{Li}^{1} = 0
\]

**Energy Conservation**

\[
\rho C_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + q^{m}
\]

\[
q^{m} = j_{Li}^{1} \left( \phi_s - \phi_e - U + T \frac{\partial U}{\partial T} \right) + \sigma_{eff} \nabla \phi_s \cdot \nabla \phi_s + \kappa_{eff} \nabla \phi_s \cdot \nabla \phi_e + \kappa_{D}^{eff} \nabla \ln c_s \cdot \nabla \phi_e
\]

- Pioneered by John Newman group at University of 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 LIBs known as the Multi-Scale Multi-Domain (MSMD) model that addresses the interplay among the physics in varied scales. Extend the porous electrode modeling:

I. Introduces multiple computational domains for corresponding length scale physics
II. Decouples LIB geometries into separate computational domains
III. Couples physics using the predefined inter-domain information exchange
IV. Selectively resolves higher spatial resolution for smaller characteristic length scale physics
V. Achieves high computational efficiency
VI. Provides flexible & expandable modularized framework

The model quantifies the impacts of the electrical/thermal pathway design on uneven charge-discharge kinetics in large format wound prismatic cells.
Developing CAE Battery Modeling Tools

I. Realizing the need to develop computer aided engineering (CAE) tools, US DOE initiated CAEBAT project in 2010

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

III. With technical support from NREL and ORNL, 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 integral part of FLUENT 15 and 16
CAEBAT Tools for Battery Design

CAEBAT tools can:

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 Modeling

Origin of mechanical failure within the active material

Crack orientation

Deformed Geometry of the fractured region
Battery Crush and Thermal Runaway

I. Battery crush may lead to failure of separator in a way that positive and negative elements may come into contact.

II. Upon contact between the positive and negative elements, currents may flow; depending on the magnitude of current and resistance on its path heat is generated.

III. Amount of heat generated depends on the cell chemistry and current and resistance between positive and negative elements.

IV. If the heat generated is not rejected in sufficient amount of time the temperature of the damaged zone may exceed the thermal runaway onset temperature.

V. After reaching the onset temperature, spontaneous reactions in the cell may continue raising the temperature potentially leading to venting, smoke, fire, and ejection of components.
Modeling Battery Mechanical Crush

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

II. In 2014, DOE initiated 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 (MECT) 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 will occur
   4. This allows us to link the mechanical aspect with the thermal aspect in a sequential fashion
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 of each representative sandwich (RS)**

- Separator 0.013mm
- Active Particles of 0.049mm
- Copper Anode of 0.025mm
- Active Particles of 0.049mm
- Active Material of 0.028mm
- Active Material of 0.028mm

**Finite element representation of one RS**

**Number of layers of each component in the RS model and battery cell**

<table>
<thead>
<tr>
<th></th>
<th>Separator</th>
<th>Positive Active</th>
<th>Positive Collector</th>
<th>Negative Active</th>
<th>Negative Collector</th>
<th>Total layers</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single RS model</td>
<td>2</td>
<td>2</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>8</td>
</tr>
<tr>
<td>One Laminate</td>
<td>22</td>
<td>20</td>
<td>10</td>
<td>20</td>
<td>11</td>
<td>83</td>
</tr>
<tr>
<td>Full Battery model</td>
<td>44</td>
<td>40</td>
<td>20</td>
<td>40</td>
<td>22</td>
<td>166</td>
</tr>
</tbody>
</table>

The RS model will be a close estimation of whole battery response.
Mechanical Simulation: Micro-scale Finite Element Model

Through thickness layout of one battery laminate

Due to symmetry, a quarter of the geometry is used to save computational time.

Each individual layer has the same in-plane mesh, and one element through the thickness.
Compression: uniform element size (0.25mm)
Indentation: multi-zone meshing

Dimensions of the battery quarter model:
Length: 25 mm
Width: 15 mm
Thickness: 4.702 mm
Battery type: 2 Ah NMC Cell

Initially, we used LS-DYNA, a general-purpose finite element program to simulate nonlinear and transient dynamic problems (http://www.lstc.com/products/ls-dyna).
LS-DYNA Mechanical Simulation and Results

- Compression
  Top rigid wall moves down quasi-statically

- Indentation
  Rigid sphere wall moves down quasi-statically

Battery Model
Bottom rigid walls fixed

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

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.
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 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).

Current density contour and vector
Electric field
Electric loading
Indentation deformed shape
Sphere Indentation on a Quarter RS model
The default adiabatic (perfectly insulated) thermal boundary condition is used. The present model can also evaluate the change of temperature during the crush. The simultaneous simulation results indicate that the temperature shows an increasing tendency during the crush, which is very likely due to increase of electric field and current density.

At present, only Joule heating is considered in the thermal analysis; more effects will be included in future work. The temperature profiles from the sequential simulation may not be as accurate as in simultaneous simulation, as heat transfer is a continuous behavior.
Linking Deformed Geometry in a cell to electrochemical-thermal models in CAEBAT
Proposed Approach for Linking Mechanical to ECT

**Initial Geometry**

**Crush Simulations in LS-DYNA**

**Export Deformed Mesh to ANSYS**

**Compute individual resistances**

**Perform ECT Simulations**

**Advantage:**
Better integration of electrical simulations with existing 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

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

I. Electrochemical-thermal tools under CAEBAT-1
   1. DOE initialed 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 crush (under CAEBAT-2)
   1. 2nd phase of CAEBAT is focusing on simulation crash-induced crush
   2. Incorporating all cell layers, a refined representative sandwich (RS) model is built;
   3. The RS model is able to capture the global stress-strain response and predict the local deformation of each component;
   4. At the sub-cell level, an anisotropic constitutive model was developed and calibrated against experiments.
   5. We also have developed a methodology to capture evolution of contact area during the short-circuit.
   6. 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 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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