A multi-scale thermal model of a high-power LiFePO$_4$ lithium-ion cell

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Introduction and goals

- Battery performance and lifetime are influenced by temperature
- Risk of fire and explosion at high $T$
- Thermal stability vital for safety and cost
- Thermal modeling is an effective tool for predicting cell thermal behavior
- A complete thermal model consists of a heat generation model and a heat transport model
- Goal: Study the temperature and heat flow patterns of a LiFePO$_4$-based cell under variable loads

Multi-scale approach

- A multi-scale thermal model for a LiFePO$_4$ lithium-ion cell is developed
- Heat transport in single cell:
  - ~20 mm scale
- Li$^+$ charge transport in electrolyte:
  - ~100 µm scale
- Li transport in solid phase:
  - ~100–1000 nm scale

Model equations

**Electrochemical model**

Thermodynamics

$$\frac{\partial \rho}{\partial T} + \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} + \frac{\partial (\rho w)}{\partial z} = 0$$

Kinetics

$$i = F \left( \frac{zF}{RT} \left( \frac{d\phi}{dx} - \frac{\partial \phi}{\partial x} \right) \right)$$

Solid-state transport

$$\frac{\partial \phi}{\partial t} + \frac{\partial \psi}{\partial t} = \frac{\partial \eta}{\partial x}$$

Electrolyte transport

$$\frac{\partial \psi}{\partial t} + \frac{\partial \sigma}{\partial t} = \frac{\partial \eta}{\partial x}$$

Heat Generation

$$Q_{\text{heat}} = Q_{\text{electrolyte}} + Q_{\text{chemical}}$$

**Heat transfer model**

- 3D finite element model using ANSYS
- Heat inside the cell

$$\rho C_p \frac{\partial T}{\partial t} + \rho \frac{\partial (uT)}{\partial x} + \rho \frac{\partial (vT)}{\partial y} + \rho \frac{\partial (wT)}{\partial z} = \nabla \cdot (k \nabla T) + Q_{\text{heat}}$$

- Heat transfer out of the cell

$$Q_{\text{out}} = \nabla \cdot (k \nabla T) + Q_{\text{heat}}$$

Assumptions:
- Jellyroll modeled as a single material with distinct thermal properties
- Variations in different directions ignored
- Effects of current collector perturbations ignored

Parameters:
- Thermal conductivity and heat capacity were determined experimentally

Multi-scale simulation

- Vertical (indirect) and horizontal (direct) coupling used for interaction

**Vertical coupling**

Start

- Electrochemical model
- Heat transfer model

Finish

**Horizontal coupling**

Start

- Electrochemical model

Finish

Simulation results

- Heat generation obtained from electrochemical simulation used as input load for heat transfer model
- Temperature distribution inside and outside the cell
- Minimum and maximum temperature profiles obtained from heat transfer simulations
- Linearly interpolated contours of heat generation from electrochemistry model used as input heat source for heat transfer model

Conclusions

- Model found to be useful in predicting thermal behavior of the cell under variable loads
- Small gradient of temperature was observed in axial direction as compared to the radial direction
- Improve parameterization of model
- Validation of the model with experimental findings
- Expand the model to be used with variable boundary conditions
- Expand the model to module level

Future work