A multi-scale thermal model of a high-power $LiFePO_4$ lithium-ion cell

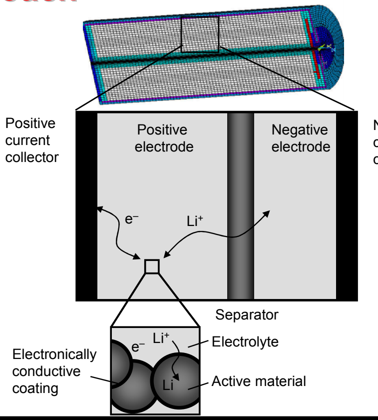
M. W. Tahir[1,*], C. Hellwig[2], C. Merten[1], W. G. Bessler[2]
1) University of Stuttgart, Institute of Chemical Process Technology (ICVT), Stuttgart, Germany
2) German Aerospace Center (DLR), Institute of Technical Thermodynamics, Stuttgart, Germany
*Email: tahir@icvt-uni-stuttgart.de

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

$$\Delta\phi_{eq}(c_{Li}) = \frac{\Delta G}{zF} = \frac{\Delta H(c_{Li}) - T\Delta S(c_{Li})}{zF}$$

Kinetics

$$i = i_0\left(\exp\left(\frac{\alpha F}{RT}\eta_{act}\right) - \exp\left(-\frac{(1-\alpha)F}{RT}\eta_{act}\right)\right)$$

$$\eta_{conc} = \frac{RT}{zF}\ln\left(\frac{c_0}{c(t)}\right) \quad \eta_{act} = \Delta\phi(t) - \Delta\phi_{eq}(c_{Li}) - \eta_{conc}$$

Solid-state transport

$$\frac{\partial\rho_{Li}}{\partial t} = \overbrace{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 D\frac{\partial\rho_{Li}}{\partial r}\right)}^{\text{Diffusion}} - \overbrace{\frac{M_{Li}}{zF}i}^{\text{Chemistry}}$$

Electrolyte transport

$$\frac{\partial(\varepsilon c_i)}{\partial t} = \overbrace{\frac{\partial}{\partial y}\left(D_i\frac{\partial c_i}{\partial y}\right)}^{\text{Diffusion}} + \overbrace{\frac{z_i F}{RT}\frac{\partial}{\partial y}\left(D_i c_i\frac{\partial\phi}{\partial y}\right)}^{\text{Migration}} + \overbrace{M_i\dot{s}_i^V}^{\text{Chemistry}}$$

$$\sum_i (c_i z_i) = 0$$

Heat Generation $Q_{total} = Q_{elchem} + Q_{ohm}$

Heat transfer model

- 3D finite element model using ANSYS

Heat transfer inside the cell

$$\rho C_{p_{cell}}\frac{\partial T_{cell}}{\partial t} = \nabla\cdot(\lambda_{cell}\nabla T_{cell}) + Q_{total}$$

Heat transfer out of the Cell

$$Q_{total} = h_f A(T_{cell} - T_{env})$$

Assumptions:

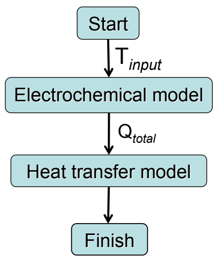
- Jellyroll modeled as a single material with distinct thermal properties
- Variations in θ direction ignored
- Effects of current collector perturbations ignored

Parameters: Thermal conductivity and heat capacity were determined experimentally

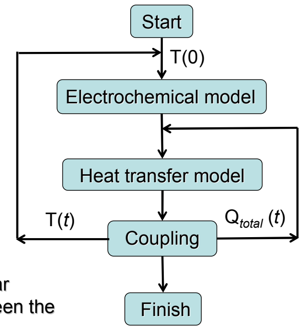
Multi-scale simulation

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

Vertical coupling

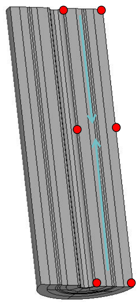


Horizontal coupling



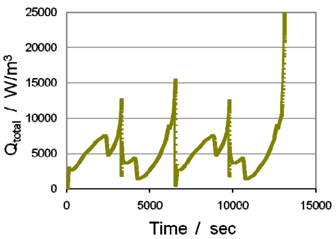
- In horizontal coupling linear interpolation is used between the representative points

Representative locations

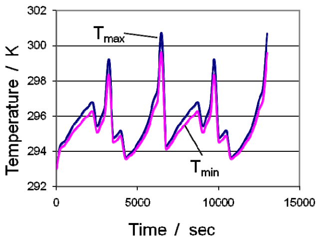


Simulation results

Vertical (indirect) multi-scale coupling

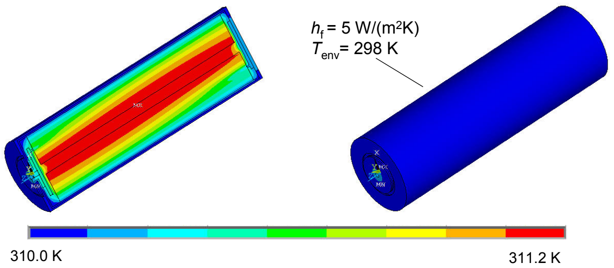


- Heat generation obtained from electrochemical simulation used as input load for heat transfer model

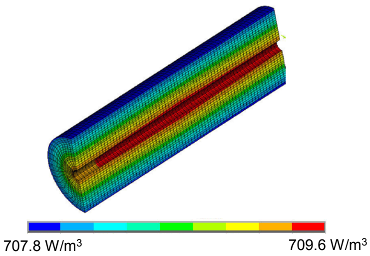


- Minimum and maximum temperature profiles obtained from heat transfer simulations

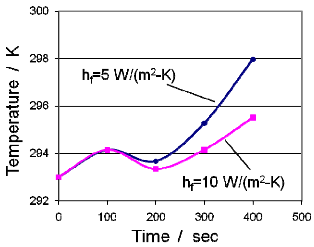
- Temperature distribution inside and outside the cell



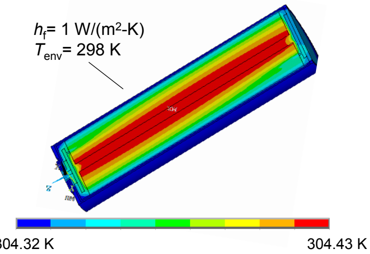
Horizontal (direct) multi-scale coupling



- Linearly interpolated contours of heat generation from electrochemistry model used as input heat source for heat transfer model



- An example simulation result showing surface temperature versus time at 5C-rate using two different boundary conditions with T_{env} = 298 K



- An example simulation result showing temperature distribution over half cell geometry at 2C-rate

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

Future work

- 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