Model development and validation of a lithium-ion pouch cell with LCO/NCA blend cathode

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The use of blend electrodes in lithium-ion cells allows to tune macroscopic properties such as rate capability, energy density and lifetime towards application requirement. Yet, the relationship design-performance relationship of such electrodes becomes highly complex. Numerical simulations and mathematical modelling are useful techniques to help understand the nonlinear processes within the cells [1].

Here we present the modelling, parameter identification, and validation of a commercial 0.35 Ah high-power lithium-ion pouch cell with LCO/NCA blend cathode and graphite anode. The transport model is based on a 1D+1D+1D (pseudo-3D or P3D) multi-scale approach [2]. Heat transport in the through-cell direction (1D, macroscale) is modeled as conductive process, mass and charge transport on the electrode-pair scale (1D, mesoscale) as diffusion and migration and intraparticle transport of lithium atoms (1D, microscale) as Fickian diffusion with concentration-dependent diffusion coefficient. The electrochemistry model allows to couple an arbitrary number of different active materials and their charge-transfer reactions, representing blend electrodes and/or electrodes with particle size distribution. The model is implemented in the in-house multiphysics software package DENIS, the electrochemistry is based on CANTERA [3].

Model parameters are identified by a combination of both literature data from similar cells (half-cell data, solid-state and liquid-phase transport coefficients) and own experimental analyses (electrochemical impedance spectroscopy, T over t, V over C during CCCV cycles). The validity of the model is demonstrated over a wide range of parameters for CCCV charge/discharge curves with different C-rates (0.05…10) and temperatures (5 °C…50 °C) as well as impedance behavior of the cell with different SOC levels (0 %…100 %) and temperatures (5 °C…50 °C). The simulations allow to identify distinct discharge regimes for the two cathode materials (LCO and NCA) and to quantify their individual contributions to overall cell impedance.

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References:

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