Modeling and Simulation of Thermal Runaway in Cylindrical 18650 Lithium-Ion Batteries

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Abstract

The thermal runaway of a single lithium-ion battery (LIB) in larger battery package is the worst case scenario which must be avoided under all circumstances. In this work the electrochemical-thermal model for a LIB based on porous electrode theory is extended with contribution coming from exothermic side reactions to model the abuse mechanisms in Li-Ion batteries with respect to the temperature which could lead to a thermal runaway. The electrochemical-thermal model is extended with several new contributions which occur in several temperature regimes. In detail the heat source in the corresponding heat equation is extended with the heat generated by various exothermic reactions, for example at the surface-electrolyte interface, reactions between anode/cathode and the electrolyte and the destruction of the electrolyte above the temperature. These extensions will be modeled with a solid fuel or a constant fuel model as simplification coming from combustion theory. For this extended model simulations are performed for specified current profiles and exterior temperature profiles to simulate an oven trial and cell cycling. For this purpose a battery model of a Lithium-Ion cell based on the Battery and Fuel Cells Module of COMSOL Multiphysics® software is extended. In the simulations a cylindrical 18650 LIB is investigated with a LiCoO2 cathode. The purpose of the simulations is to compute the temperature-field during the time evolution of a thermal runaway, therefore the cross section in horizontal and vertical direction are considered as well as the one-dimensional temperature profiles along these directions. Finally the time evolution of the overall mean cell temperature T is used to classify the different stages of a thermal runaway in a "T-dT/dt" plot. The results will be compared with experimental ARC-measurements in pure oven experiments and cycling experiments.

Reference

[1] A. Melcher et al., Modeling and Simulation of the Thermal Runaway Behavior of Cylindrical Li-Ion Cells—Computing of Critical Parameters, Energies, Vol. 9, p. 292 (2016)
[2] A. Melcher et al., Modellierung und Simulation des thermischen Runaways in zylindrischen Li-Ionen Batterien, Tagungsband ASIM-Treffen STS/GMMS, pp. 8-28 (2016)

Figures used in the abstract

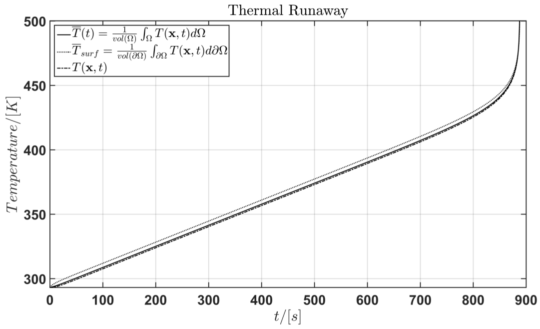

Figure 1: Thermal Runaway.