Multi-scale Simulation of Thermo/Electrochemical Mechanism in Li-ion Cells at Elevated Temperature

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Thermal runaway of lithium ion cells is one of critical issues for practical operation of large-scale cells [1]. As a pilot study preliminary to building an early-alert heat management system for Li-ion cells, we present 1D multi-scale simulation of a single cell with calculation of side reactions occurred at elevated temperature in addition to simulation of normal operating conditions. The thermo-electrochemical model used in this work is designed to understand electrochemical and thermochemical kinetics in range from micro to macro scales [2]. Lithium insertion and extraction through active materials are assumed to follow Butler-Volmer kinetics.

Two different kinds of cells are compared to investigate contributions to temperature rises by thermodynamic potentials of each type of cathode: lithium iron phosphate (LiFePO\(_4\), LFP) and blends of lithium manganese oxide (LiMn\(_2\)O\(_4\), LMO) spinel with lithium nickel cobalt aluminum oxide (LiNiCoAlO\(_2\), LNCA). Thermodynamic potentials, entropy and enthalpy of lithiation, of LFP are referred from work done by Dodd [3]. The potentials for the blends are obtained by applying weighting factors to potentials of pure LMO and LNCA based on experiments by Tran et al. [4]. The thermodynamic potentials and kinetic of the blend cell are validated by comparison with experimental discharge curves in 0.1, 1, 5 and 10 C rate at 303, 313 and 333K (Fig. 1).

As for thermochemical side reactions at elevated temperature, we include exothermic decomposition of SEI and EC (e.g. formation of SEI) and cathode/MCMB anode in various C rates at room temperature.

**References**


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**Fig. 1.** Comparison between simulation and experiment of discharge curves for LMO spinel/LNCA mixture cathode/MCMB anode in various C rates at room temperature.

**Fig. 2.** Cell average temperature profile and heat flow from anode of self-heating by SEI formation and decomposition with full cell model at constant ambient temperature of 400K.