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Multi-scale Simulation of Thermal Runaway and Cell-to-cell propagation in Lithium-ion Battery Packs: Impact on Ni content and SOC based on DSC Kinetics

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Thermal runaway (TR) in lithium-ion batteries (LIBs) poses significant safety risks, particularly at the module and pack level where cell-to-cell (CTC) thermal propagation can lead to catastrophic failures. While a multitude of factors contribute to the thermal behavior and runaway of LIBs, this study specifically isolates and investigates the impact of two critical parameters: cathode Nickel (Ni) fraction and State of Charge (SOC), on TR susceptibility and its subsequent propagation dynamics. This study aims to develop a multi-scale simulation model to predict TR behavior and CTC propagation within battery modules and packs, integrating cell-level thermal properties derived from Differential Scanning Calorimetry (DSC) data for cathodes with varying Ni contents and SOC levels. Initially, cell-level thermal behavior was characterized using DSC for cathode materials with varying nickel (Ni) fractions across different SOCs. Key kinetic parameters governing exothermic reactions were extracted from the DSC data. These parameters informed an individual cell thermal model, which was subsequently integrated into a comprehensive module and pack-level multiphysics simulation framework. This framework explicitly models coupled phenomena such as heat transfer pathways between adjacent cells and other relevant pack components, enabling the analysis of neighboring cell impacts. The results demonstrate that cell-level instabilities, exacerbated by higher Ni content and SOC as indicated by DSC, directly translate to increased risks at the pack level. The multi-scale/multiphysics simulation quantifies how these two selected factors (Ni fraction and SOC) influence the propensity, speed, and extent of CTC propagation, predicting critical metrics such as time delays between cell failures and the number of affected neighboring cells. This work presents a robust methodology linking DSC-derived cell kinetics (specifically related to Ni content and SOC) to module- and pack-level safety performance through multiphysics modeling, providing a valuable tool for assessing the impact of these particular aspects of cell chemistry and operational state on CTC propagation risk, while also aiding in the design of safer battery packs with improved thermal management.