Experimental and Modeling Investigation on Nail-Penetration-Induced Thermal Runaway of Lithium-ion Batteries with Different States of Charge

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Thermal runaway (TR) remains a critical safety challenge for lithium-ion batteries (LIBs), necessitating advanced diagnostic and modeling approaches to elucidate its dynamic evolution for early detection and mitigation. This study first experimentally investigates the multidimensional signal evolution of 18650-type $Li(Ni_{1/3}Co_{1/3}Mn_{1/3})O_2$ (NCM) cells with varying states of charge (SOC) during nail penetration-induced TR. Experiments are conducted in a sealed combustion chamber equipped with a motor-driven nail penetration system and a Schlieren optical setup, enabling synchronized capture of gas venting and combustion dynamics. Multidimensional signals, including recoil force, voltage, pressure, temperature, Schlieren imaging of gas venting and combustion, and final gas composition, are measured. Optical diagnostics are employed to quantify key gas venting and combustion parameters, such as venting velocity, venting angle, and flame propagation speed.

The results indicate that, across all tested SOCs, the TR process follows five distinct stages: nail penetration, gas venting, smoke obscuration, flame propagation, and flame extinction. Among all measured signals, optical diagnostics and recoil force exhibit the fastest response to TR, followed by pressure, voltage, and temperature signals. Due to the high gas venting velocity, shock waves are observed near the safety valve in cells with SOCs ranging from 50% to 120%, with a maximum venting velocity of 232 m/s recorded in the 120% SOC case. During gas venting, jet fire behavior is observed in cells with SOCs above 70%, featuring flame propagation speeds an order of magnitude higher than those at 50% SOC condition.

To further interpret the observed TR phenomena and quantify the influence of SOC on hazard severity, a multi-physics computational model is developed using COMSOL Multiphysics™. The model incorporates multiple heat sources, including internal short-circuit (ISC)-induced ohmic heating and exothermic side reactions, to simulate the temperature rise during TR. Moreover, a self-developed chemical kinetic mechanism [1] is integrated to describe gas generation during TR. To characterize the gas venting process following safety valve opening, a lumped model is proposed to estimate venting velocity. The simulation results reproduce key features of the TR process observed experimentally, including the onset time of venting, flame speed, and maximum flame temperature. This modeling framework provides a deeper understanding on TR dynamics and supports predictive evaluations for battery safety design.

References

[1] Zhang J, Ma C, Liu S, Guo Q, Liu S, Han P, Huang Z, Han D. Chemical Reaction Neural Networks to Map Lithium-ion Battery Thermal Runaway Gas Generation. Cell Reports Physical Science. 2025, 102563.