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A Coupled Thermal-Electrical Model for Lithium-Ion Battery Thermal Runaway with Gas Generation and Venting Dynamics

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Thermal runaway (TR) in lithium-ion batteries (LIBs) remains one of the most critical barriers to their safe deployment in electric vehicles and grid-scale energy storage. In this work a comprehensive, experimentally validated, model is developed to simulate thermal runaway (TR) and venting in lithium-ion pouch cells, with NMC-based cathode, where TR is initiated by external heating. It is based on a previously developed coupled electrical-thermal model that included the initial energy input, the chemical decomposition processes of the anode, cathode and the electrical energy released by an internal short circuit and currently extended to include gas generation, internal pressure and venting dynamics. The current model covers the full TR evolution — from the triggering event (external heating / internal short circuit) through multistage chemical decomposition, to pressure build-up and the ejection of gas. The model captures key features of TR, such as temperature evolution and temperature change rate, internal pressure changes and reproduces the characteristic-venting mechanism, whereas triggering energy, internal short-circuit resistance ratio, electrolyte combustion, and anode decomposition heat were identified as the dominant parameters controlling TR severity. Five distinct TR severity clusters are identified spanning no-TR to severe thermally triggered TR, with electrolyte combustion found to be the single most decisive factor for reaching the most severe outcome. Its findings are expected to support the foundation for future research dedicated on improving battery safety, as it provides a quantitative platform for battery safety design, test-protocol optimisation, and thermal propagation risk assessment.

The model spans initiation (external heating / ISC), multistage chemical decomposition, pressure build-up, venting dynamics. Despite the selected continuously varied parameters, TR events naturally group into five clusters from no-TR to severe TR, indicating that the governing physics create discrete qualitative regimes rather than a continuum. Triggering energy, separator breakdown temperature, and NMC activation energy are the three most influential parameters. Cell chemistry and cooling design matter most in the moderate-combustion regime. Electrolyte combustion is decisive. The ratio E_NMC-I/E_eva is the single most important material-level parameter. When close to unity, severe TR is unavoidable; when close to 2, mild TR is the expected outcome. Hard ISC at low energy is most reproducible.

For standardised testing, initiating TR via hard ISC at the lowest possible additional thermal energy gives the most repeatable and reproducible outcome.