Flammability and Explosion Features of Lithium-Ion Batteries: effect of Cathode Chemistry and State of Charge

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The IEA predicts that global electricity consumption will increase between 2025 and 2027, mainly driven by industrial activity in China, the U.S., and India. This trend highlights the need for advanced and reliable energy storage solutions. Lithium-ion batteries, commonly used in consumer electronics, electric mobility, and renewable-powered smart grids, are central to addressing this growing demand. Selecting the appropriate cathode is essential to battery performance and safety, influencing energy capacity and stability. Common materials include lithium cobalt oxide (LCO), lithium iron phosphate (LFP), lithium nickel manganese cobalt oxide (NCM), and lithium nickel cobalt aluminium oxide (NCA), typically coated on an aluminium current collector. NCM and NCA offer high energy but pose thermal risks due to nickel content. In contrast, LFP provides superior safety, longevity, and cost-effectiveness, making it ideal for risk-sensitive applications. However, If not properly managed, lithium-ion batteries can be subject to various forms of abuse and misuses, such as overheating, mechanical impact, overcharging, or failures in the battery management system. These events can lead to internal short circuits and activation of rapid exothermic reactions, potentially triggering thermal runaway. During thermal runaway, hazardous gases are released into the atmosphere, including CO_2/CO, flammable gases (H_2, CH_4, C_2H_4, C_2H_6), and toxic compounds like HF and POF_3. The accidental ignition of these gases may lead to fires and/or explosions. According to UL 9540A, assessing the flammability and explosion characteristics of the released gases is essential for designing effective prevention and mitigation measures. The aim of this work is to characterise the hazard of batteries as function of cathode chemistry and state of charge (SOC). Flame speed, deflagration index, maximum pressure, flammability limits, radical production, and sensitivity analysis were conducted for various cathodes and SOCs using CHEMKIN simulations. In Figure 1 the deflagration index is plotted as function of the equivalence ratio, as computed for different cathodes. NCA, NMC90505, and LFP release greater quantities of hydrogen and carbon monoxide, resulting in higher deflagration indexes compared to LCO and lower-nickel NMC chemistries.

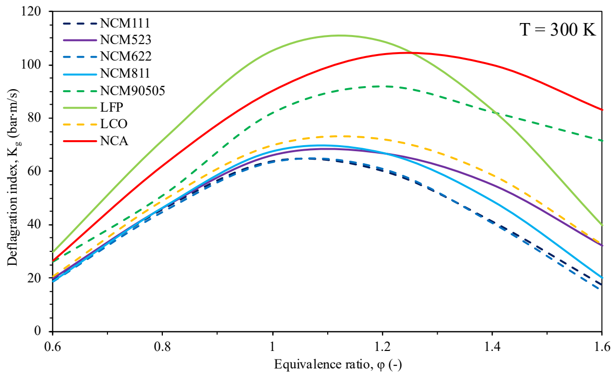

Fig. 1. Deflagration index as a function of equivalence ratio for battery vent gas compositions from various cathode chemistries

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