A Lithium Battery Model Using Non-equilibrium Thermodynamics for Heterogenous Systems

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Understanding and managing battery temperature is crucial for optimizing the performance, lifespan, and safety of lithium-ion batteries. We model the lithium-ion battery (LIB) using the theory of non-equilibrium thermodynamics for heterogeneous systems NETH [1].

The battery is divided into five subsystems: the two bulk electrodes, the two electrode surfaces and the bulk electrolyte. The surfaces are described with Gibbs excess properties. The electrolyte consists of a lithium salt ($LiPF_6$) and two organic carbonates (DEC and EC). The electrodes are lithium intercalated graphite (anode) and LCO (cathode), which corresponds to a conventional LIB [2]. The work can be seen as an extension of the work of Spitthoff et al. [3]; it is a full model using NETH. Thanks to Gullbrekken et al. [4], further transport properties are now available to describe the coupling of electric current, heat and mass transport in the electrolyte. The integration of these properties into the extended NETH cell model revealed additional contributions to the uneven temperature distribution within the cell.

The electrode surfaces act as a heat source or heat sink, depending on the direction of the electric current flow. In an exemplary temperature profile during steady-state conditions for a single cell, incorporating Peltier heats of -137 kJ/mol and 49 kJ/mol for the anode and cathode surfaces, respectively, we can observe a temperature rise at the anode surface of about 0.0018 K . The boundary temperatures are fixed and the current density is 30 A/m^2, which corresponds to a 1 C discharging rate [3]. In the context of a single cell, the observed temperature changes are insignificant. However, as demonstrated by Spitthoff et al. [3], these minor changes accumulate to a substantial temperature shift when multiple cells are stacked, by raising the temperature in the center by roughly 8 K. This finding underscores the importance of understanding and managing temperature variations, especially when dealing with stacked cells. Deviations from a uniform temperature distribution can have significant implications for battery management systems.

Moreover, an analysis of the cell's entropy production reveals that the predominant contribution emanates from the surfaces. This observation suggests that a more profound understanding of surface properties has the potential to significantly enhance the optimization of the overall lost work within the cell. In essence, improving our knowledge of surface characteristics can play a pivotal role in minimizing energy losses and enhancing the efficiency of the cell.

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References

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