From electrode dynamics to protocol design: a multiscale approach to fast charging of Li-ion batteries

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The widespread adoption of electric vehicles (EVs) is critically dependent on the development of lithium-ion batteries that can support rapid charging without compromising long-term durability. Within the broader context of chemical engineering, this challenge calls for the integration of advanced modelling, materials characterisation, and electrochemical diagnostics to inform the design of robust and efficient charging strategies. In this study, we address this need by developing a non-equilibrium thermodynamics phase-field model[1,2] to investigate and control degradation phenomena arising during fast charging of commercial graphite/NiMnCo cylindrical cells. The model couples lithium intercalation kinetics with the dynamics of phase separation in graphite, a key factor in triggering parasitic reactions at high current densities. A rigorous calibration and validation campaign is carried out using a combination of experimental techniques, including full-cell electrochemical tests (0.1C–2C), impedance spectroscopy, and structural characterisation of electrode materials. The resulting model is employed to design a physics-informed fast-charge protocol that achieves an 80% state-of-charge within 15 minutes while mitigating degradation. Compared to standard industrial protocols, both manufacturer-specified and those implemented in commercial EVs, the proposed strategy demonstrates superior performance in terms of charge time and cycle life. Long-term cycling over 500 iterations confirms a capacity retention exceeding 95%, highlighting the effectiveness of model-guided approaches in bridging the gap between battery electrochemistry and practical system operation. This work exemplifies the potential of chemical engineering methodologies, particularly those combining modelling, experimentation, and optimisation, to tackle multidisciplinary challenges in sustainable energy storage.

Keywords: *physics-based modelling, phase-field, model-informed design, fast-charge, Li-ion battery*

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