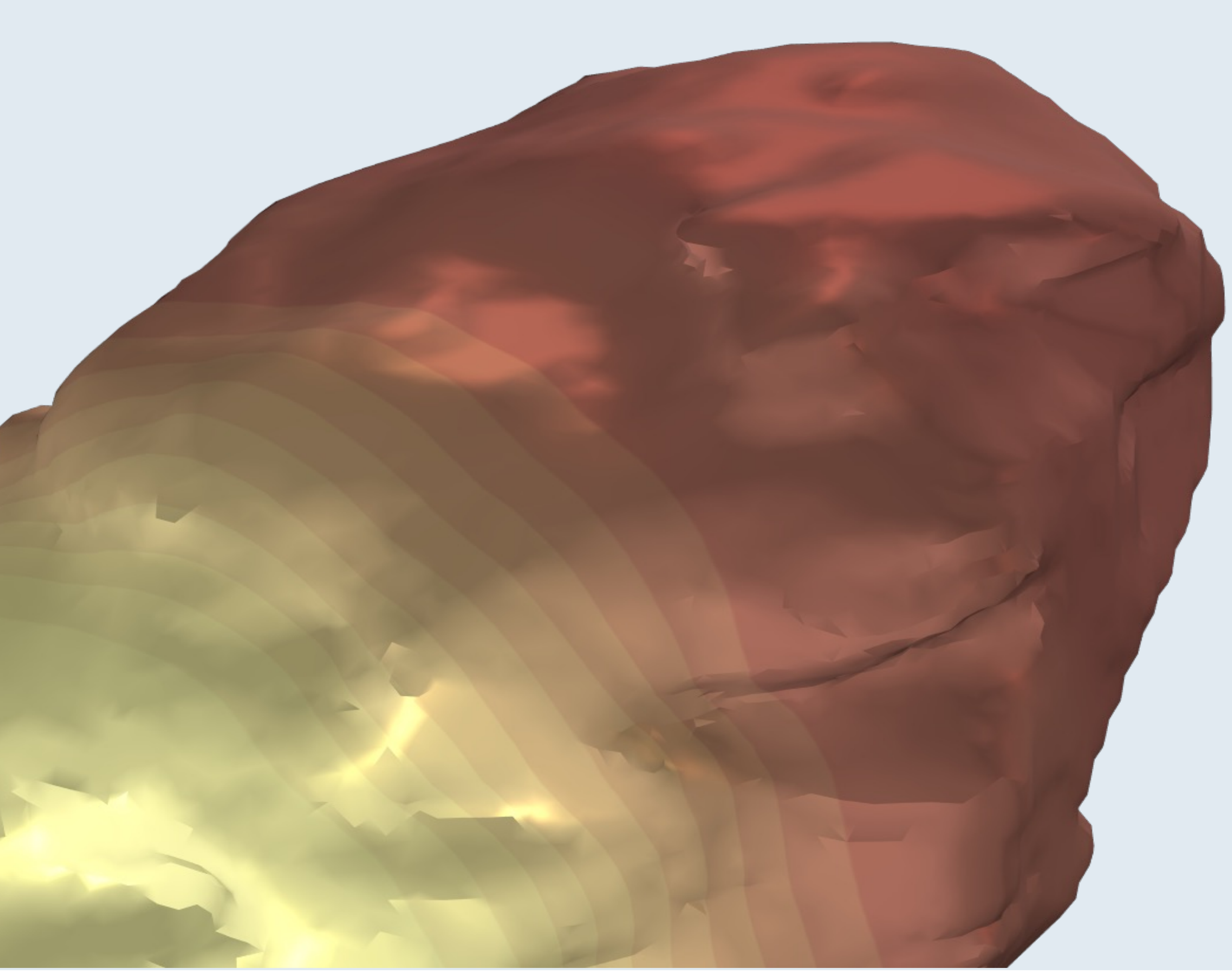

Advanced Modelling for Li-ion Battery Design, Diagnostics and R&D

Predicting cell behavior during intense operation conditions requires advanced physics-based models incorporating intercalation dynamics and accounting for degradation phenomena.

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Introduction

Lithium-ion batteries are leading the electrification transition, particularly in electric vehicles (EVs). However, fast charging emerges as a major concern for the customers. The design of charging protocols and the related diagnostics of battery state-of-health require a physics-based model. The model must account for the dynamics of lithium intercalation in graphite, which phase-separates into several Li-rich and Li-poor domains (called stages), as well as the interplay with the major degradation phenomena, including the deposit of metallic lithium on top of graphite (lithium plating) and the growth of a resistive decomposition layer called solid electrolyte interphase (SEI).

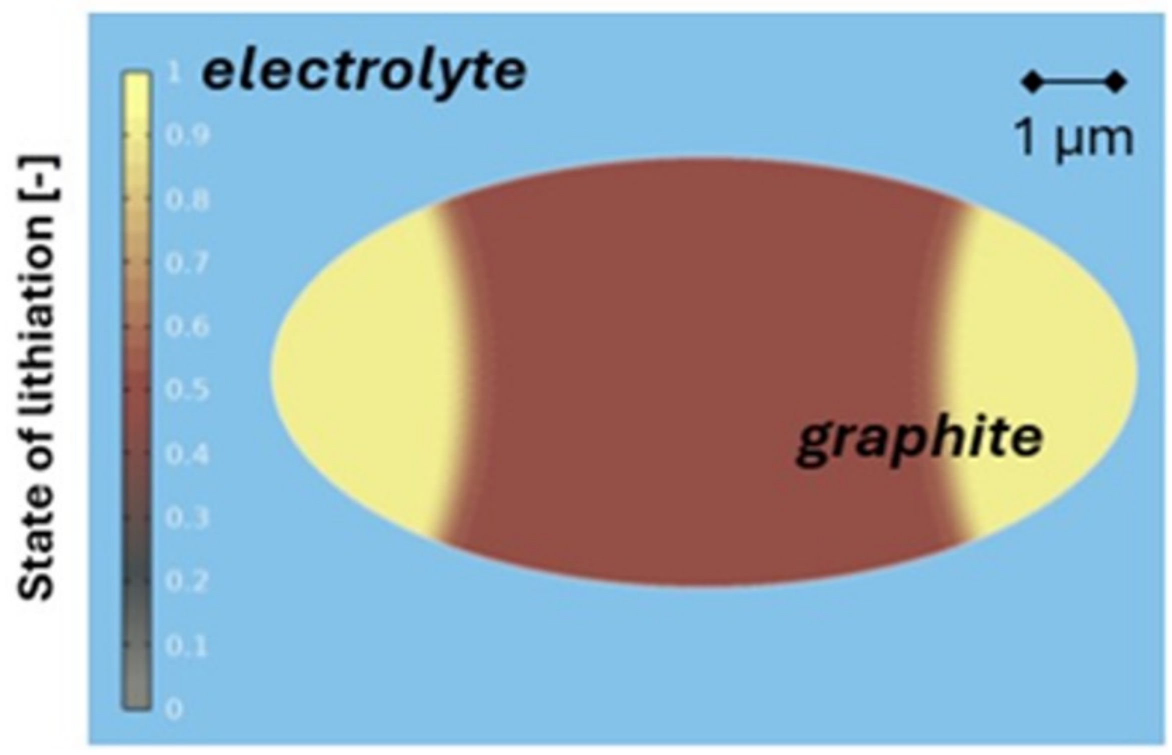

FIGURE 1. Phase-separation in Li-rich and Li-poor phases in a graphite particle simulated via phase-field modelling.

Methodology

We integrated a phase-field approach (Figure 1), rooted on non-equilibrium thermodynamics, within pseudo-2D and 3D modelling frameworks[1-3]. The molar balance of intercalated lithium becomes a fourth-order partial differential equation since the chemical potential depends on the Laplacian of concentration. This is conveniently implemented as two coupled second-order equations in the General Form PDE interface. In-house kinetic expressions of Li plating, Li stripping, and SEI growth are included as boundary ODEs and DAEs.

Results

By using the model, the main bottlenecks during charge can be predicted and avoided. By monitoring the activation overpotential of Li plating and SEI growth, the current (in terms of C-rate) is modulated to complete the battery charge in less than 15 minutes between 20% and 80% state-of-charge (Figure 2). Special attention is given to avoid the evolution of degradation phenomena especially at the end of the charge, resulting in a smaller final cell potential and applied current.

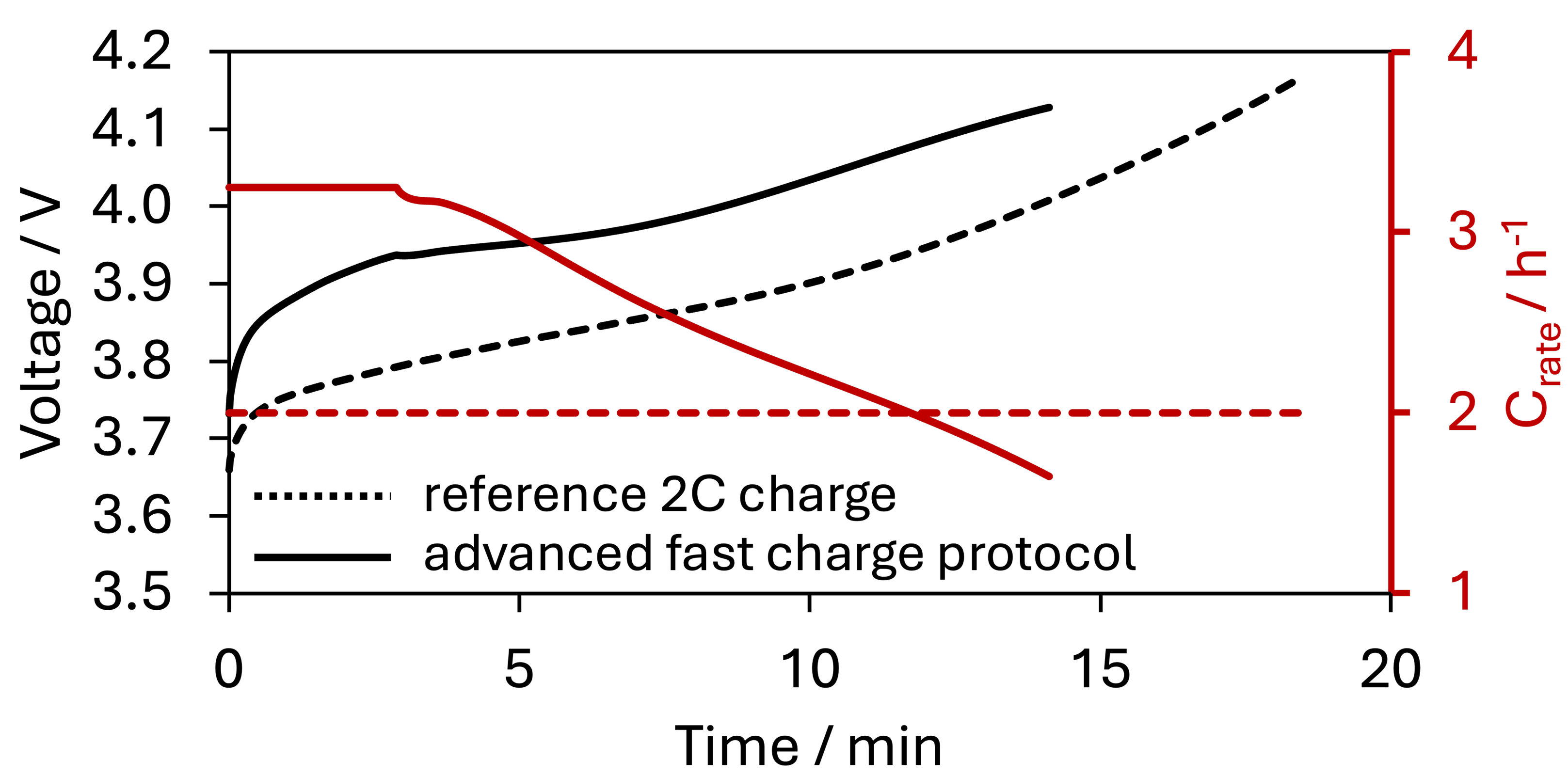

FIGURE 2. Comparison of an advanced fast charge protocol conceived by the model and a reference 2C charge.

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