Comparing Common Zero-dimensional SEI Models Under Varied Conditions

Effects of Initial State of Charge, C-rate, and Charge-Discharge Asymmetry

Kawa Manmi*, Ferran Brosa Planella

Mathematics Institute, University of Warwick, Gibbet Hill Road, Coventry, CV4 7AL, United Kingdom

*kawa.manmi@warwick.ac.uk

Abstract

The solid electrolyte interphase (SEI) is critical for battery performance but poorly understood. This research compares common zero-dimensional SEI models to analyse:

- Initial SOC effects on SEI growth
- C-rate impacts on growth patterns
- Charge vs discharge asymmetry

Our findings provide insights into model behaviour under different conditions and highlight limitations in capturing experimental observations.

Introduction

SEI formation significantly impacts:

- **Manufacturing:** 25-32% of production costs
- **Performance:** Battery lifetime, safety, capacity

Experimental evidence shows SEI growth is significantly higher during charging than discharging.

"An ideal SEI requires high ionic conductivity, high electronic resistivity, mechanical stability, and chemical stability"

Methods

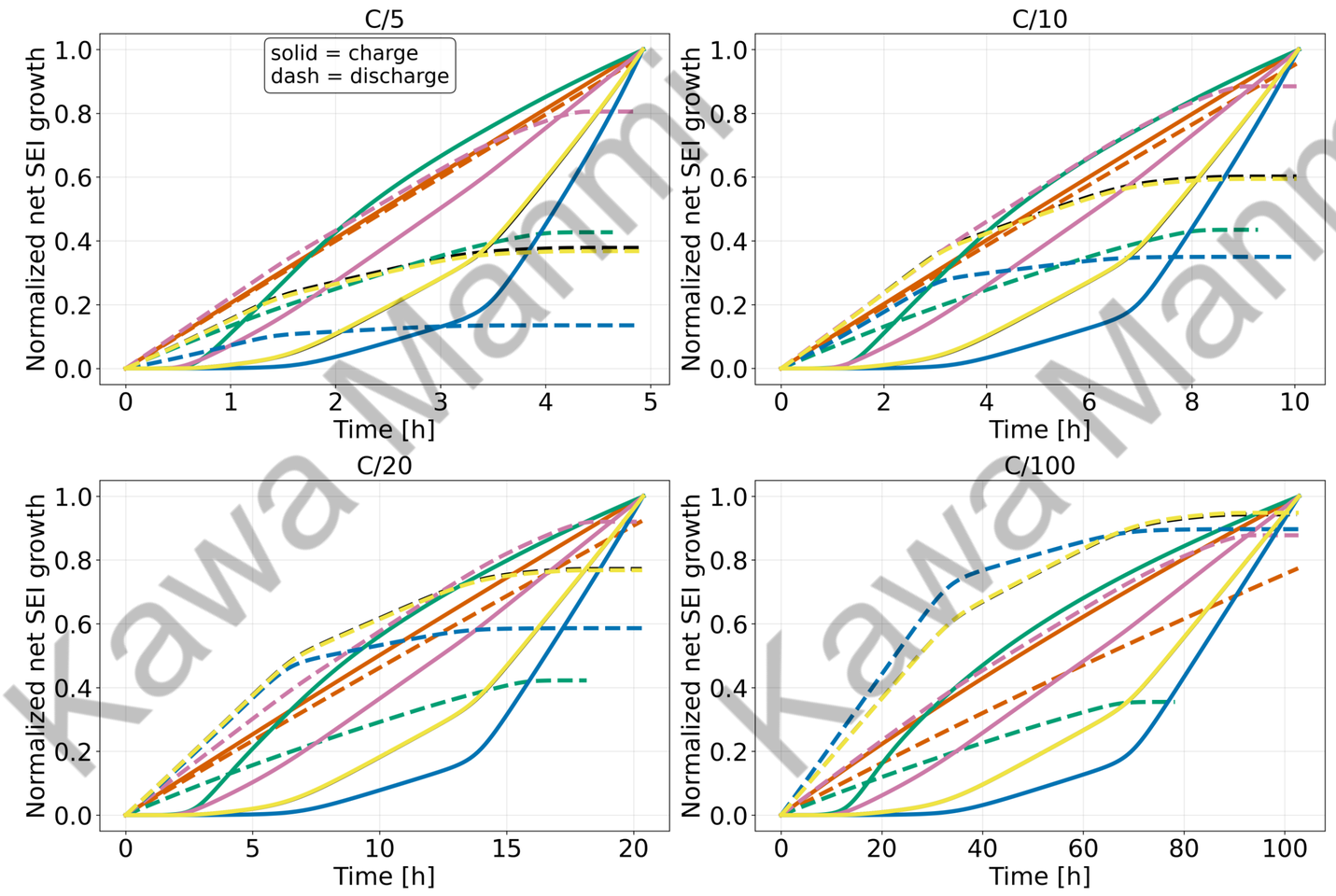
We analysed all SEI models in PyBaMM:

Reaction limited	Solvent-diffusion
EC reaction	Electron-migration
Interstitial-diffusion	Von Kolzenberg

Key parameters varied:

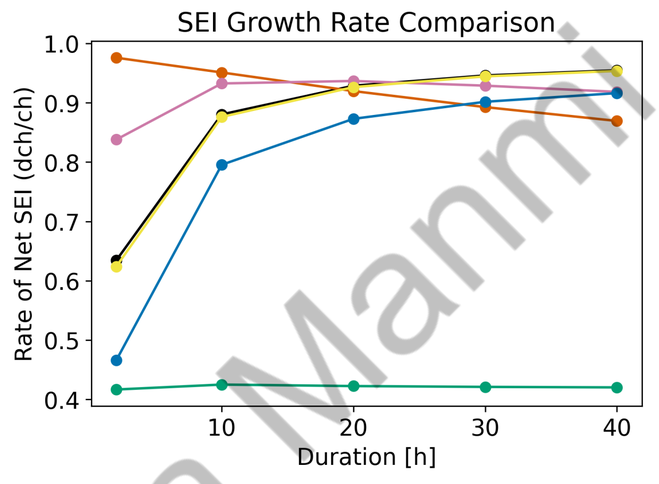
- C-rates: C/5 to C/100
- Initial SOC: 0.1 to 0.9
- Charge vs. discharge conditions

Charge vs. Discharge Asymmetry Across Different C-rates



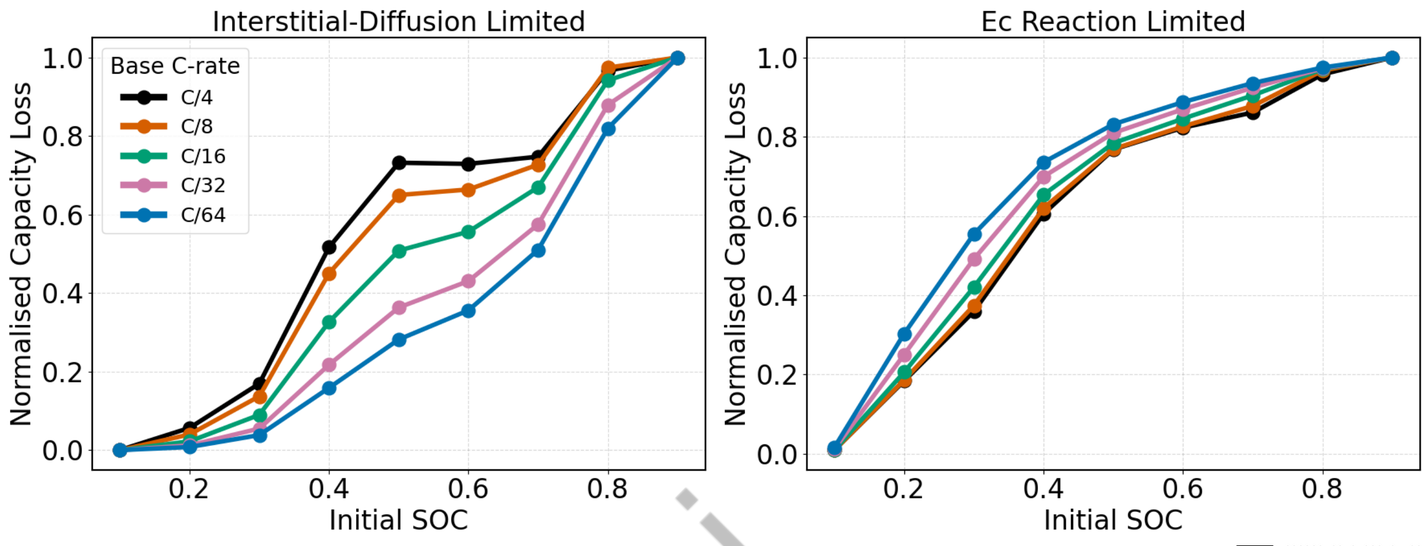
- All models show higher SEI growth during charging than discharging
- At lower C-rates (C/100), some models show more symmetric behaviour

Extended Duration Protocol Effects



- Protocol: Matched charge/discharge durations at C/300 reveal time-dependency of SEI formation rather than C-rate dependency
- Ratio of discharge/charge SEI growth approaches 1.0 (symmetry) with increased duration for most models
- Duration of hold is more important than C-rate for achieving symmetry.
- This suggests time-dependent mechanisms dominate over rate-dependent ones

Initial SOC Effects



- Discharge tests used adjusted C-rates to fully discharge from each initial SOC value
- Higher initial SOC leads to more SEI growth across all models.
- Interstitial-diffusion shows non-linear relationship while EC reaction model shows consistent behaviour regardless of C-rate.

References

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Researcher bio

Kawa is a Faraday Institution Research Fellow at the University of Warwick, focusing on physics-based mathematical modelling of battery SEI layer formation and growth. He completed his PhD in Applied Mathematics (University of Birmingham, 2015) and has extensive experience in numerical fluid dynamics. He contributes to PyBaMM, an open-source battery modelling software.

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PyBaMM

Faraday Battery Challenge Delivered by Innovate UK