A physics-informed Neural Network based on an electrochemical model to estimate the battery capacity

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Abstract

Most existing state-of-health (SOH) estimation methods are largely empirical, offering limited insight into the actual electrochemical processes governing battery degradation, whether they rely on equivalent-circuit models or purely data-driven techniques. This lack of physical interpretability remains a central challenge in reliable SOH prediction. Physics-Informed Neural Networks (PINNs) address this gap by embedding fundamental electrochemical laws directly into the learning process, ensuring that predictions remain physically meaningful. In this work, we employ a PINN-based framework that integrates a mechanistic degradation model capturing four dominant aging pathways: solid-electrolyte interphase (SEI) growth, lithium plating, loss of active material (LAM), and other secondary degradation mechanisms. By explicitly linking these physical processes to capacity fade, the proposed approach estimates capacity loss over the entire cycle life in a consistent and interpretable manner. Under constant C-rate cycling conditions, the model achieves an RMSE below 0.05, outperforming conventional empirical methods while providing clearer physical insight, highlighting the critical role of physics-guided learning in improving SOH prediction.

Ⅰ. Introduction

Lithium-ion batteries are the backbone of modern technology, powering everything from smartphones and laptops to electric vehicles, spacecraft, drones, and large-scale energy storage systems. Their widespread adoption stems from a unique combination of long cycle life, low weight, and high energy density. However, different applications impose very different demands. Engineers working with chemistries such as LFP, NMC, and NCA must constantly trade off energy density, safety, cost, and durability. For example, drones favor lightweight cells with high specific power, stationary storage systems prioritize stability and longevity, and EVs demand long driving range along with fast-charging capability. Across these use cases, batteries are exposed to harsh operating conditions such as extreme temperatures, high C-rate charging and discharging, mechanical vibrations, and strict safety constraints.

Because of these diverse operating conditions, battery aging pathways strongly depend on both chemistry and usage. LFP cells, for instance, are generally more thermally stable but can degrade rapidly under overcharge, while NMC cells may suffer from structural instability at high voltages. Accurately capturing such complex, chemistry-specific degradation behavior is essential for reliable cycle-life prediction and performance optimization. Modeling approaches span a broad spectrum. Physics-based electrochemical models and mechanistic degradation frameworks, such as P2D models, provide deep insight into processes like loss of active material, SEI evolution, lithium plating, and stress-induced fracture [1], but they are computationally expensive and rely on well-identified parameters. On the other hand, data-driven methods—including SVMs, Gaussian processes, random forests, and deep neural networks—can achieve strong predictive accuracy using voltage and current data, yet often struggle outside their training domain and lack physical interpretability.

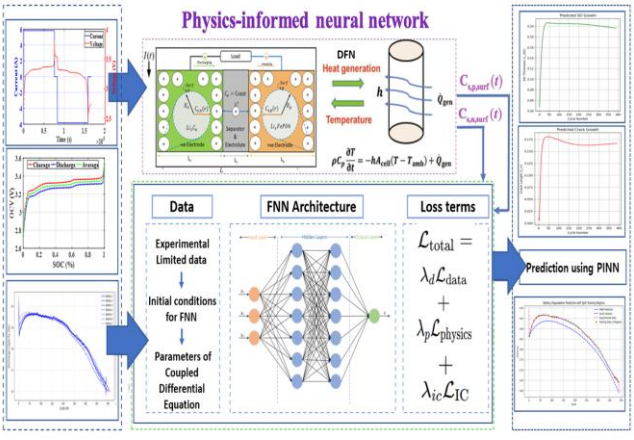


Fig. 1. The PINN framework combines experimental data with DFN-based thermal-electrochemical physics.

Hybrid approaches, especially Physics-Informed Neural Networks (PINNs), bridge this gap by embedding physical laws or constraints directly into the learning process, enabling data-efficient training, improved generalization, and even the identification of dominant degradation modes without requiring extensive end-of-life labels.

In this study, we take a hybrid approach as shown in Fig. 1, estimating capacity fade across cycle life by integrating key degradation pathways—SEI growth, lithium plating, LAM, and auxiliary side reactions—into a PINN framework. This aims to produce reliable, interpretable SOH predictions across chemistries and operating situations by striking a compromise between mechanistic knowledge and data efficiency.

Ⅱ. Method

We model long-term capacity fade using a reduced, DFN-inspired mechanistic core embedded within a Physics-Informed Neural Network (PINN). Rather than solving the full set of electrochemical PDEs during inference, the framework evolves three physically meaningful degradation states on a per-cycle basis SEI layer thickness L, plated-Li thickness δ_{Li}, and the remaining active-material fraction f_{act}. Their dynamics are written as ODEs that serve as PINN residual constraints as shown in Equation [1].

$$\frac{dQ}{dn} = \theta k_{wet}(A_{\max} - A_{eff}) - \frac{\partial L_{SEI}}{\partial n} - \frac{\partial \delta_{Li}}{\partial n} - \frac{\partial f_{act}}{\partial n} \qquad (4)$$

The neural backbone takes cycle index and operating/context features (e.g., C-rate, temperature) and predicts the latent states and capacity, while the loss combines data misfit with the ODE residuals.

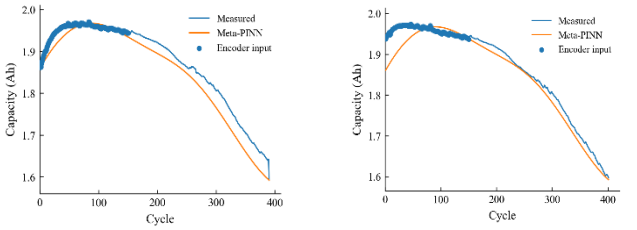
Ⅲ. Results and discussion

Batch 1 (2C charge / 1C discharge, 7 cells) Across 400 cycles, the PINN maintains consistently low error below 0.03 Ah for all cells (0.021 ± 0.006 Ah), whereas the physics-only model gradually drifts to 0.30– 0.38 Ah and the purely data-driven NN reaches 0.13– 0.56 Ah. The parameters inferred by the PINN suggest moderate crack growth(K_{cr} = 3.9×10^{-20} m²/s), limited lithium plating ($i_{0,pl}$ = 4.3×10^{-9} A·m^{-2}), and comparatively higher solid-phase diffusivity(D_{sol} = 9.3×10^{-22} m²/s consistent with stable aging behavior Fig [2a].

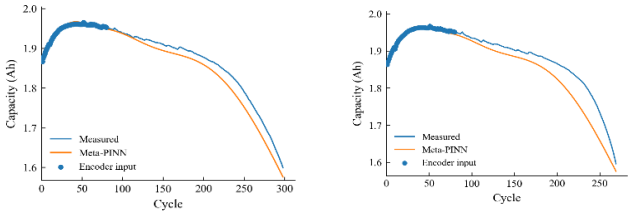
Batch 2 and Batch 3 (3C charge / 1C discharge, 15 cells each). With faster charging, degradation accelerates and the weaknesses of baseline models become more pronounced: the NN exhibits large error spikes exceeding 1 Ah for several cells, while the physics model reaches about 0.18 Ah error. In contrast, the PINN remains robust, keeping errors within 0.05 Ah (≈ 0.026 ± 0.010 Ah). The learned parameters indicate that the dominant change under higher C-rates is enhanced lithium plating, reflected by a ~40% increase in ($i_{0,pl}$ = 6.1×10^{-9} A·m^{-2}) while crack growth remains nearly unchanged and solid diffusivity slightly decreases(D_{sol} = 7.8×10^{-22} m²/s) as shown in Fig [2b-c].

Ⅲ. Conclusion

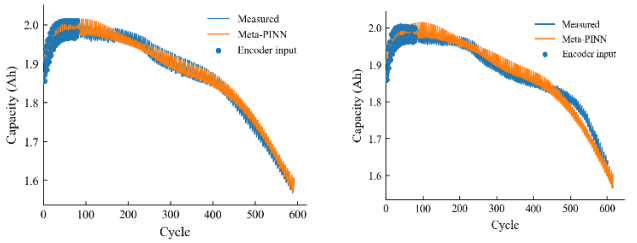
For NCM cells, our PINN forecasts capacity fade with RMSE < 0.05 Ah—over an order of magnitude lower than both a calibrated physics model and a black-box neural network. A lightweight, cell-specific encoder, conditioned only on the first 10 cycles, infers key kinetics (e.g. plating exchange current, crack-growth rate) without manual retuning, and these estimates remain consistent across varied NCM formulations.



(a) Capacity prediction of two 2 C NMC cells; PINN matches experiment, baselines deviate late-cycle.



(b) Capacity-retention curves for two 3 C NMC cells; PINN follows data, physics and NN diverge.



(c) Capacity prediction of two X C {X: 0.5, 1, 2, 3, 5} of fully discharged cells.

Fig. 2. PINN capacity predictions for six NMC cells under different cycling protocols.

This mechanistic fidelity enables real-time health monitoring: BMS digital twins can use the model to adapt charging profiles, thermal control, and maintenance scheduling on the fly. In sum, minimal early-cycle data plus embedded physics yields accurate, generalizable predictions and actionable diagnostics for NCM durability.

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REFERENCES

[1] S. E. J. O'Kane et al., "Lithium-ion battery degradation: how to model it," Physical Chemistry Chemical Physics, vol. 24, no. 13, pp. 7909– 7922, Mar. 2022