

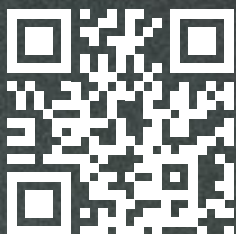


Data-driven and hybrid ageing models

PHYSICS-INFORMED FEATURE ENGINEERING AND FOUNDATION-MODEL-BASED STATE OF HEALTH (SOH) PREDICTION IN NEMO'S BATTERY MANAGEMENT SYSTEM

As part of Key Exploitable Result 5 (KER 5), VUB MOBI develops data-driven and hybrid ageing models for battery State of Health (SoH) estimation. The data-driven pipeline extracts physics-informed features from electrochemical measurements and feeds them into a tabular foundation model (TabPFN). The hybrid extension adds parameters fitted by a physics-based P2D electrochemical model (COMSOL Multiphysics) as additional inputs, directly linking degradation mechanisms to the predictor.

Discover how EIS, incremental capacity analysis, and physics-model parameters combine to achieve more accurate and interpretable SoH predictions across diverse ageing conditions and real-world driving profiles.



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Research approach

Feature engineering from electrochemical data

- Incremental capacity analysis (ICA) from quasi-OCV curves (LEAN method) captures peak height, shift and area-under-curve signatures linked to loss of lithium inventory and active material.
- EIS-derived resistance signatures capture ohmic, charge-transfer, and diffusion behaviour across the ageing trajectory.
- Operational descriptors — temperature, depth of discharge, C-rate, elapsed time — contextualise electrochemical behaviour across conditions.

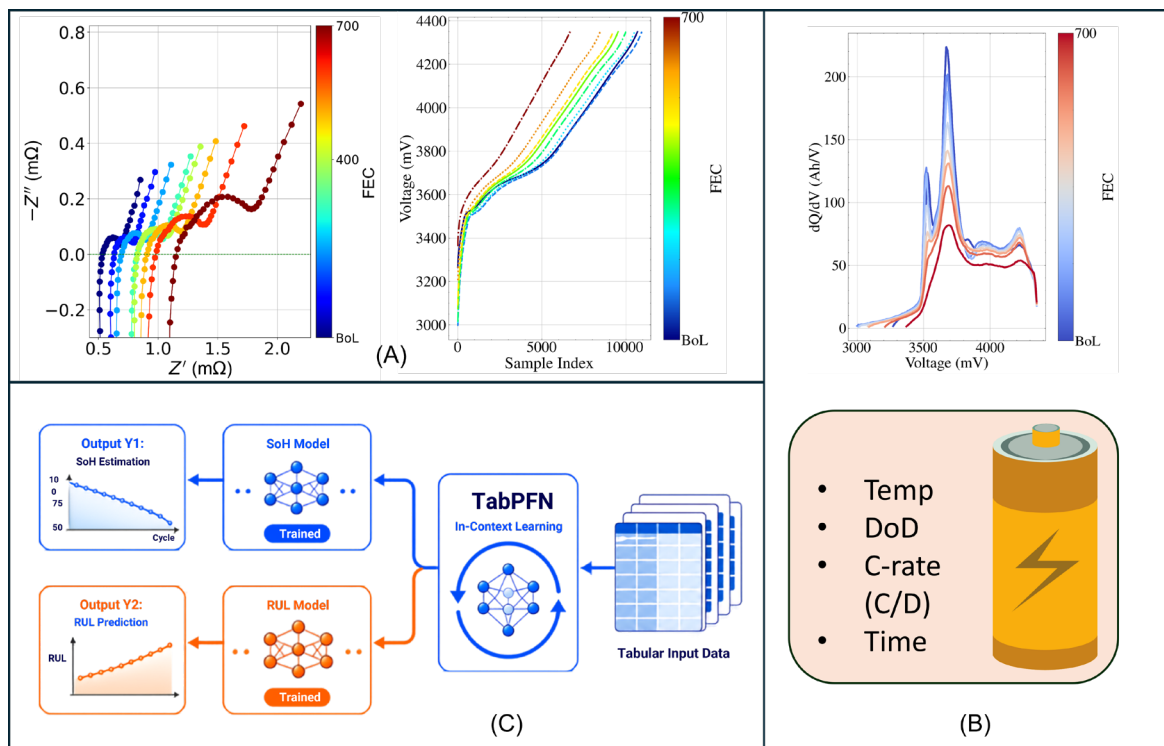
Feature selection & foundation-model prediction

- An mRMR algorithm combined with AutoML selects a compact, non-redundant feature subset.

- TabPFN performs multi-output SoH prediction via in-context learning across 16 cycling conditions spanning 5°C, 25°C and 45°C, multiple DoD windows, C-rates, and a WLTC driving profile.

Hybrid ageing model

- A feature-level hybrid couples the WP3 physics-based (COMSOL Multiphysics) P2D model with the TabPFN data-driven predictor: physically meaningful parameters fitted to EIS measurements are supplied alongside experimental features as model inputs.
- From 13 physics parameters, 4 are selected that directly reflect key degradation mechanisms: EC (electrolyte conductivity), κ_{film} (SEI-film conductivity), κ_{C} (CEI-film conductivity), and D_n (solid-state lithium diffusion).
- Each additional physics parameter configuration was tested incrementally; all improved on the pure data-driven baseline, with the four-process combination achieving the best overall performance.



Feature extraction and TabPFN-based modelling framework for SoH and RUL prediction.

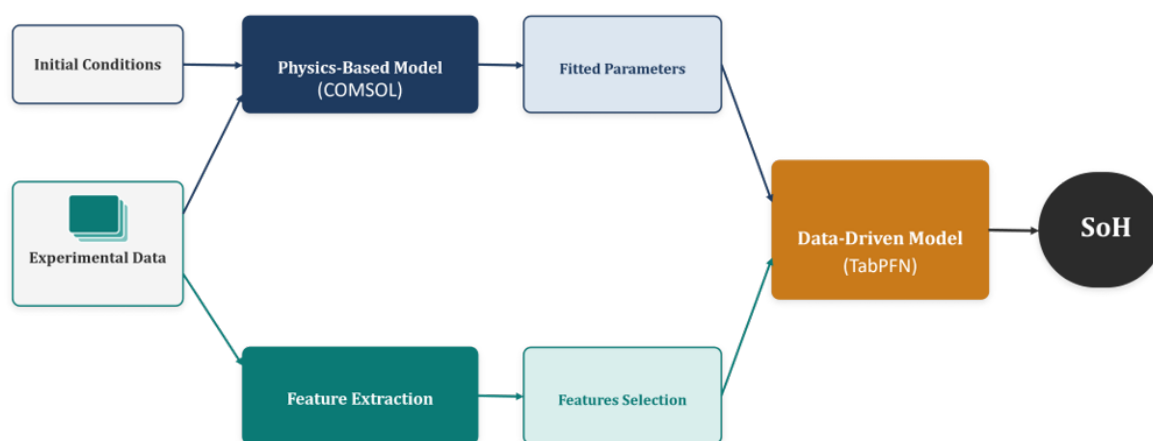
Key Findings

Data-driven SoH estimation

- ◆ A compact set of IO diagnostic EIS and cycling features is sufficient for accurate SoH tracking.
- ◆ Average MAE of 0.63% and R^2 of 0.97 across validation cells at 5°C, 25°C and 45°C, covering both first-life (>80% SoH) and second-life (<80% SoH) regimes.
- ◆ Under the dynamic WLTC profile, the model generalises from constant-current training data: MAE of 0.45% and R^2 of 0.85.

Hybrid model findings

- ◆ The physics-based P2D model (COMSOL Multiphysics) was validated for one cycling condition (DoD 100%, IC/IC, 45°C); the hybrid evaluation is therefore limited to that same condition and is not directly comparable to the multi-condition data-driven results above.
- ◆ On that single test condition, adding the four physics parameters as inputs improves all three metrics relative to the pure data-driven baseline on the same condition: R^2 rises by +5.01%, MAE falls by -23.18%, and MAPE falls by -23.21%.
- ◆ CEI-film conductivity (κ_C) produced the largest individual MAE reduction among the four parameters; combining all four degradation-linked descriptors delivered the best overall performance.
- ◆ Physics-based features compensate for limited training data: with just one cell's data, the pure model accumulates error at beginning of life (0 FEC), while the hybrid model reduces this by anchoring predictions to electrochemically-meaningful parameters.



Hybrid modelling workflow: COMSOL Multiphysics physics parameters and experimental features feed jointly into the TabPFN data-driven predictor for SoH estimation.

Take-away

Physics-informed feature engineering and a pre-trained tabular foundation model (TabPFN) enable accurate SoH prediction across 16 diverse cycling conditions, including dynamic WLTC profiles. Where physics-model parameters are available, adding them as hybrid inputs further reduces MAPE by over 23% on the same test condition, linking predictions to interpretable degradation mechanisms.