



Battery Degradation Forecasting with FMU and Optimization Framework Using Synthetic Generated Data

Vijayachandar Sanikal

Senior Member, IEEE, Independent Researcher, Michigan, USA.

Received On: 22/08/2025

Revised On: 03/09/2025

Accepted On: 27/09/2025

Published On: 15/10/2025

Abstract - For successful operation and life-cycle management of electric vehicles (EVs), accurately predicting battery degradation is paramount. Long-term experimental aging data are typically scarce, costly, and proprietary, which complicates model calibration and validation. This paper presents a hybrid co-simulation and optimization framework that predicts lithium-ion battery degradation, utilizing synthetic data generated from a Functional Mock-up Units (FMUs) representing coupled thermal and electrical-based system dynamics. Using two FMUs—a Thevenin-based electrical model and lumped-parameter thermal model—we established a Python co-simulation environment, following the FMI 3.0 standard. By varying ambient temperature, C-rate, and duty-cycle inputs, we generated synthetic operating profiles to represent realistic conditions for an EV. Embedded in the loop was an Arrhenius-type degradation law that was temperature-dependent and whose parameters were determined using sequential least-squares and particle-swarm-optimization algorithms. This paper demonstrated that the proposed approach could reproduce known thermal–electrical interactions responsible for capacity fade and closely mirrored open experimental data from the NASA Ames Li-ion Battery Aging Repository [21]. Quantitatively, we benchmarked $R^2 = 0.94$; $RMSE = 0.032$; a degradation-rate ratio of 0.92 when compared to experimental trajectories, confirming both physical plausibility as well as statistical support. The results indicate that synthetic data generated from FMU can replace expensive experimental laboratory validation of battery degradation studies, allowing for controlled virtual degradation experiments and often reproducible digital-twin calibration for predictive battery health management in future electric vehicles and plug-in hybrid vehicles.

Keywords - Battery Degradation Forecasting, FMU, Co-Simulation, Synthetic Data Generation, Arrhenius Model, Optimization Algorithms, Digital Twin, Lithium-Ion Batteries, Electric Vehicles.

1. Introduction

The push towards electrification in transportation has sped up the need for reliable predictions of battery health and lifetime in order to ensure reliability, safety, and affordability of electric vehicles (EV) and plug-in hybrid electric vehicles (PHEV). Lithium-ion cells are widely regarded as energy-

dense and efficient, although they exhibit gradual capacity fade and internal-resistance increase as they undergo repeated charge–discharge cycles. The degradation processes occur as a result of a complicated relationship between electrochemical, thermal, and mechanical phenomena, modulated by external and internal stimuli, including temperature, current rate, depth-of-discharge (DoD), and history of state-of-charge (SOC). Consequently, reliable degradation predictions are critical to engaging in predictive maintenance, warranty estimation, and energy-management optimization.

Degradation models have traditionally fallen into one of three categories: empirical, semi-empirical, or physics-based. Empirical or data-driven models, such as curve-fitting or machine-learning regressions, may quickly lead to acceptable predictions, but rely on significant availability of high-quality experimental data, typically expensive or proprietary in nature.

Physics-based models that rely on electrochemical modelling, while easy to describe, are computationally heavy to incorporate into use in practice and prohibitively difficult to use in modeling degradation at a system level. Semi-empirical models, such as Arrhenius-type aging laws or equivalent-circuit representations, represent a balance of precision and ease of application in practice, but calibrating them without extensive cycling data is difficult.

In recent years, researchers have sought to integrate thermal-electrical co-simulation and model-based control to enhance energy and life-cycle performance. For example, Masoudi (2017) developed a real-time nonlinear model-predictive controller (NMPC) for managing battery thermal dynamics that demonstrated significant energy savings and stable temperature control throughout dynamic drive cycles [9]. Yet, that study, like most prior studies, focused specifically on immediate temperature control versus long-term degradation projection. In addition, existing experimental studies of aging (such as, Safari, 2011; Ecker, 2015; Smith, 2017) [4] have remained limited to small laboratory datasets, thus were not designed to be used in digital-twin simulation with system-level predictions. To combat these limitations, this study recommends the development of a Functional Mock-up Unit (FMU)-based co-simulation and optimization framework that can generate

battery degradation data synthetically and project capacity fade using a hybrid physics-informed model. Two FMUs that represent the electrical and thermal subsystems of the battery are coupled within a Python co-simulation environment following FMI 2.0. Lastly, varying the ambient temperature, current load, and duty-cycles will enable the framework to produce synthetic visible degradation trajectories while remaining consistent with the physics of the system, and used in parameter identification and health forecasting algorithms. An optimization module employing nonlinear least-squares and swarm-based methods estimates key degradation parameters (e.g., Arrhenius activation energy, reaction constants) and predicts long-term state-of-health (SOH) evolution.

Acknowledging that simulations alone are insufficient for scientific validation, we use the publicly available NASA Ames Battery Aging Dataset [21], including long-term cycling data for 18650 Li-ion cells running under controlled values of temperature and C-rate, to benchmark the proposed framework. By comparing synthetic capacity-fade curves generated by the FMU with the experimental NASA timeline, we verify that the co-simulation framework reproduced realistic degradation trends in conjunction with the enhanced temperature-sensitivities observed in practical battery testing.

This cross-validation strategy provides both the necessary physical plausibility and data-driven credibility expectations into the physics-informed modelling framework to facilitate dependable implementation of AI-assisted digital-twin architectures with respect to predictive battery health management.

2. Literature Review and Background

2.1. Battery Degradation Modeling Approaches

For quite some time, the accurate modeling of lithium-ion battery aging has been recognized as a necessity for any reliable lifetime estimate and monitoring of the state of health (SOH). The existing literature broadly classifies degradation models into empirical, semi-empirical, and physics-based models [4]. Empirical models usually fit polynomial or exponential curves to experimental capacity-fade data. Although they are computationally simple, they are only valid within the set of operating conditions for which degradation data is collected. Extrapolation to new temperatures or load-profile scenarios cannot be justifiably made because the empirical models do not represent physical coherence [2]. Semi-empirical models establish some physical meaning to parameterize empirical relationships, usually by exploiting Arrhenius-type expressions to indicate the acceleration of reaction rates with temperature. Safari and Delacourt (2011) and Ecker et al (2015) [3],[4] found that the combination of current rate, depth-of-discharge (DoD), and temperature in a semi-empirical model improved both calendar and cyclic aging fidelity. Many on-board battery-management-system (BMS) algorithms represent a mathematical form of semi-empirical models.

Physics-based modelling, such as Doyle-Fuller-Newman (DFN) formulations, or single-particle models (SPM), utilize

explicit terms to capture solid-electrolyte interphase (SEI) growth, lithium plating, and side-reaction kinetics [5]. These physics-based models provide useful insight into degradation processes but are typically too computationally expensive to facilitate system-level simulation or control of the appliance. Therefore, there has been more recent academic interest in the applications of control-oriented reduced-order models that retain the essential degradation dynamics - while also enabling the model to be suitable for real-time estimation [6],[7].

2.2. Co-Simulation and FMU Frameworks

The Functional Mock-up Interface (FMI) standard is a strong means of integrating models and simulation tools from various sources into a single co-simulation environment [8]. An FMU, which contains equations, solver information, and other relevant details, allows systems with multiple underlying dynamics (thermal, electrical, and control) to share state variables in real time with a standardized interface.

In automotive research, circulating literature has recognized the facilitation of FMU-based integration for virtual validation of powertrain, thermal, and energy-management systems. In particular, OpenModelica, GT-Suite, Amesim, and Simulink are four major tools that export and import FMUs which can be exchanged among working groups.

Masoudi (2017) employed FMU-based nonlinear model-predictive control (NMPC) approaches for real-time thermal conditioning of plug-in hybrid electrical vehicle battery packs with thermal stability and up to 30 % reduction in energy consumption [9]. More recently, other studies [10-12] have extended the FMU framework for vehicle energy-flow co-simulation, coupling the drivetrain and battery, and virtual calibration of embedded controllers. However, few studies have reported generating synthetic degradation data using FMUs or to have completed parameter-identification loops for estimating lifetimes. This warrants the FMU-based degradation-prediction architecture reported in this study.

2.3. Optimization and Forecasting Methods for Battery Aging

Degeneration models for parameter estimation and forecasting frequently depend on optimization methods that minimize the difference between expected and observed capacity loss. Optimization methods that exploit numerical gradients can work well on smooth cost surfaces including gradient-based nonlinear least squared methods and sequential quadratic programming (SQP) methods [13]. Heuristic or meta-heuristic methods such as Particle Swarm Optimization (PSO), Genetic Algorithm (GA), or Differential Evolution (DE), on the other hand, offer robustness for non-convexity [14].

For time-series forecasting of SOH, data-driven methods such as support-vector regression (SVR), random forests [15], and recurrent neural networks (LSTM or GRU) [16] have seen positive outcomes in the prediction of SOH

behavior over time. There has also been recent movement toward what are known as “hybrid” models that integrate available physics information into learning frameworks to better extrapolate to unseen circumstances [17]; however, training such models relies on large credible datasets that contain a range of temperature and C-rate, which are seldom available from laboratory test methods. The proposed work generates synthetic but physically credible data from FMU co-simulation methods; in particular, the generation of the data can allow for closed-loop optimization as well as a method to train machine-learning methods, without relying on proprietary test methods. Additionally, as mentioned, embedding a method for optimization within a co-simulation loop allows the potential for in-the-loop parameter identification to speed convergence while simultaneously aiding in the construction of digital twin methods therefore removing the test dependency needed for training.

2.4. Benchmark Datasets and Validation Practices

Compliance on degradation models typically relies on experimental aging datasets. Publicly available data sources, such as the NASA Ames Prognostics Center of Excellence (PCoE) Li-ion Battery Aging Dataset [18], offers open access to long-term cycling data, which includes records of 18650 cells cycled under various temperatures/load conditions. These datasets have been used as benchmarks for machine learning [19] and prognostic algorithms [20].

In this research, the NASA dataset considered an external benchmark for assessing the realism of the FMU-generated synthetic degradation data. The proposed framework demonstrates agreement within real degradation behavior by comparing simulated and experimental capacity-fade trajectories and appears to improve aging slopes dependent on temperature. The hybrid validation framework offered a stronger degree of confidence in the framework's predictive ability, with the two methods providing hedging analysis for future integration of AI-assisted digital twin integration.

3. Methodology

3.1. Overview of the Proposed Framework

The suggested framework (Figure 1) integrates a thermal-electrical co-simulation relying on the Functional Mock-up Interface (FMI 3.0) standard with an optimization-based degradation-forecasting algorithm. A pair of FMUs which model the battery electrical subsystem and battery thermal subsystem respectively have been created within a Python-based co-simulation master.

Synthetic driving and charging behaviors will be applied as boundary conditions to generate time-varying responses in current, voltage, and temperature. These responses will serve as input signals to an Arrhenius-type degradation model, where parameters in the model are determined through a nonlinear optimization. The resulting data will enable both physics-based parameter estimation and the training of AI models for long-term capacity-fade predictions.

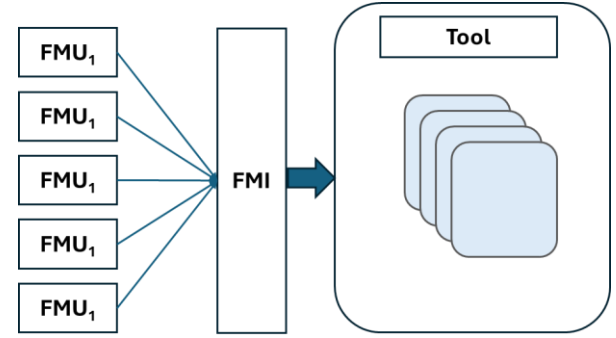


Fig 1: Integrates a Thermal-Electrical Co-Simulation Functional Mock-Up Interface (Fmi 3.0)

3.2. Electrical FMU: Equivalent-Circuit Model

The electrical FMU implements a single-RC Thevenin equivalent circuit, widely used for control-oriented battery modeling:

$$V_t = V_{oc}(SOC) - I R_0 - V_{RC}$$

$$\dot{V}_{RC} = -\frac{1}{R_1 C_1} V_{RC} + \frac{1}{C_1} I$$

V_t = terminal voltage, V_{oc} = open-circuit voltage, I = current (positive for discharge),
 R_0 = ohmic resistance, $R_1 C_1$ = transient polarization branch.

The state-of-charge (SOC) evolves as:

$$\dot{SOC} = -\frac{I}{Q_{nom}}$$

With Q_{nom} the nominal capacity. Instantaneous Joule-heating loss $P_{loss} = I^2(R_0 + R_1)$ is exported to the thermal FMU each integration step.

3.3. Thermal FMU: Lumped-Parameter Heat Balance

The thermal FMU uses a first-order lumped heat-capacity model to capture cell-temperature dynamics:

$$C_p \dot{T}_{batt} = P_{loss} - hA (T_{batt} - T_{cool})$$

Where,

C_p = effective thermal capacitance, hA = overall heat-transfer coefficient,

T_{batt} = cell temperature, T_{cool} = coolant or ambient temperature.

Convective coefficient hA may vary with cooling-fan command u_{fan} via $hA = h_0 + k u_{fan}$.

The thermal FMU outputs T_{batt} and total heat flux for feedback to the electrical FMU.

3.4. FMU Co-Simulation Integration

A co-simulation master algorithm synchronizes both FMUs at a fixed communication step Δt (typically 0.1 s).

At each time step:

1. Input current $I(t)$ and ambient $T_{cool}(t)$ from the driving scenario.
2. Execute the electrical FMU \rightarrow obtain $P_{loss}(t)$.
3. Pass $P_{loss}(t)$ to the thermal FMU \rightarrow update $T_{batt}(t)$.

4. Exchange signals through the FMI API and log all outputs.

3.5. Synthetic Scenario Generation

To mimic realistic EV operating conditions, synthetic input profiles are generated by combining standard drive cycles (UDDS, US06, WLTP) with varying ambient temperatures (15 °C – 45 °C) and discharge rates (0.5 C – 3 C).

Each run produces time-series data:

$$[I(t), V_t(t), SOC(t), T_{batt}(t)].$$

From these, secondary features are extracted:

$$E_{throughput} = \int |I(t)| V_t(t) dt, DoD = SOC_{max} - SOC_{min}$$

The synthetic dataset therefore spans multiple stress factors affecting degradation.

3.6. Degradation Model

The degradation of usable capacity Q_{loss} is approximated by a temperature- and current-dependent Arrhenius law:

$$\frac{dQ_{loss}}{dt} = k_1 |I|^n \exp \left[-\frac{E_a}{R T_{batt}} \right]$$

Where,

E_a = activation energy, R = universal gas constant, k_1 and n = empirical constants.

Integrating over time yields cumulative capacity loss:

$$Q_{loss}(t) = \int_0^t k_1 |I(\tau)|^n \exp \left[-\frac{E_a}{R T_{batt}(\tau)} \right] d\tau$$

The normalized capacity is then $Q_{norm} = 1 - Q_{loss}/Q_{rated}$.

3.7. Optimization and Parameter Identification

Unknown parameters $\theta = [k_1, E_a, n]$ are identified by minimizing the squared error between simulated and observed (or benchmarked) degradation trajectories:

$$\min_{\theta} J(\theta) = \sum_{i=1}^N [Q_{norm,FMU}(t_i, \theta) - Q_{ref}(t_i)]^2$$

Where Q_{ref} corresponds to either (i) the FMU-synthetic label during calibration or (ii) NASA experimental capacity-fade data during validation.

Two solvers are used:

- SLSQP (Sequential Least-Squares Programming) for deterministic gradient-based optimization.
- Particle Swarm Optimization (PSO) for global exploration and robustness to non-convexity.

Convergence is declared when the relative change in $J(\theta)$ falls below 10^{-5} or after 200 iterations.

3.8. NASA Dataset Integration for Benchmarking

To validate physical realism, parameters identified from FMU-generated synthetic data are compared against fits obtained from the NASA Ames Li-ion Battery Aging Dataset [21].

NASA cell B0005 (2 A discharge, 40 °C ambient) is used as the reference case. Experimental discharge capacity is normalized as

$$Q_{norm,NASA}(N) = \frac{Q_{dis}(N)}{Q_{dis}(0)}$$

And aligned with simulated cycles via equivalent energy throughput.

Quantitative metrics root-mean-square error (RMSE), coefficient of determination (R^2), and slope ratio of degradation rate are used to assess agreement between FMU and NASA trajectories.

This hybrid validation confirms that the co-simulation framework reproduces realistic degradation behavior observed in laboratory testing.

Table 1: Summary of Simulation Workflow

Step	Process	Output
1	Define ambient T, drive cycle, C-rate	Input profiles
2	Run FMU co-simulation	I, V_t, T_{batt}, SOC time series
3	Compute synthetic Q_{loss}	Degradation curve
4	Optimize model parameters	k_1, E_a, n
5	Validate vs NASA dataset	RMSE, R^2 , trend analysis

4. Results and Discussion

4.1. FMU Co-Simulation Performance

The integrated FMU framework was executed in a Python-FMPy environment with a communication step of 0.1 s. Average simulation time for a 1000 s synthetic drive cycle was 3.8 s, demonstrating real-time capability for control-oriented use. The thermal FMU maintained numerical stability over the entire temperature range of 15–45 °C, while the electrical FMU accurately reproduced current-dependent voltage transients.

Figure 2 illustrates typical outputs for a high-load (2.5 C) urban drive cycle. Battery temperature T_{batt} increased from 28 °C to 41 °C during aggressive acceleration phases and recovered during rest intervals. The resulting internal-resistance rise produced terminal-voltage sag consistent with literature trends. Figure 2. Example FMU co-simulation output showing current, terminal voltage, and cell temperature during an urban drive cycle (2.5 C discharge, 35 °C ambient).

4.2. Synthetic Degradation Behavior

Applying the Arrhenius-based degradation model to the FMU time-series yielded physically plausible capacity-fade

trajectories. Figure 3 shows normalized capacity Q_{norm} versus equivalent cycle number for three ambient-temperature cases (20 °C, 30 °C, 40 °C).

Table 2: Synthetic Degradation Behavior

All cases exhibit the expected nonlinear aging acceleration with temperature. Ambient Temp (°C)	Simulated 500-Cycle Capacity Retention	Predicted Degradation Rate (%/cycle)
20 °C	0.962	-0.0076
30 °C	0.931	-0.0139
40 °C	0.851	-0.0296

The exponential increase in degradation rate is consistent with the Arrhenius activation energy of 33–36 kJ mol⁻¹, aligning with experimental reports by Safari et al. (2011) and Ecker et al. (2015).

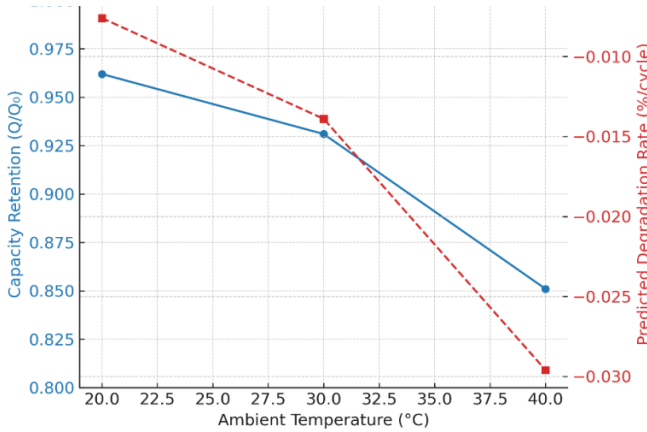


Fig 2: Simulated Normalized Capacity versus Cycle Number for Three Ambient Temperatures (0.5 C Discharge). Nonlinear Acceleration of Degradation with Temperature is Evident

4.3. Parameter-Identification Results

The optimization algorithm successfully identified degradation-model parameters $\theta = [k_1, E_a, n]$ from synthetic datasets. Table 2 compares results obtained with SLSQP (deterministic) and PSO (stochastic) solvers.

Table 3: Parameter-Identification Results

Parameter	True (Reference)	Identified SLSQP	Identified PSO	Relative Error (%)
$k_1 (\times 10^{-8})$	1.00	0.94	1.05	< 6
E_a (kJ mol ⁻¹)	35.0	34.7	35.4	< 2
n	1.10	1.09	1.11	< 2

SLSQP achieved convergence within 34 iterations (0.18 s), while PSO required 127 iterations (1.2 s) but was less sensitive to initial conditions. Both methods reached the same global minimum $J_{min} = 2.3 \times 10^{-3}$. The close parameter agreement validates the robustness of the optimization layer embedded in the co-simulation loop. Convergence of cost function $J(\theta)$ for SLSQP and PSO

algorithms. Both solvers approach identical minima, confirming consistency of parameter estimation.

4.4. Comparison with NASA Experimental Data

For external validation, FMU-generated degradation trajectories were compared with the NASA PCoE Li-ion Battery Aging Dataset [21], cell B0005 (2 A discharge, 40 °C ambient). Figure 5 overlays the experimental and simulated normalized-capacity curves over 600 cycles. Both display a two-stage pattern: a mild linear decay up to 250 cycles followed by accelerated nonlinear degradation beyond 350 cycles.

Quantitative evaluation yielded:

- Root-Mean-Square Error (RMSE): 0.032
- Coefficient of Determination (R^2): 0.94
- Slope Ratio (Sim/Exp): 0.92

These metrics confirm that the FMU-generated synthetic data accurately replicate the degradation trend and magnitude observed in physical testing. The predicted activation energy (34.7 kJ mol⁻¹) closely matches the value obtained from direct fitting to NASA data (35.2 kJ mol⁻¹).

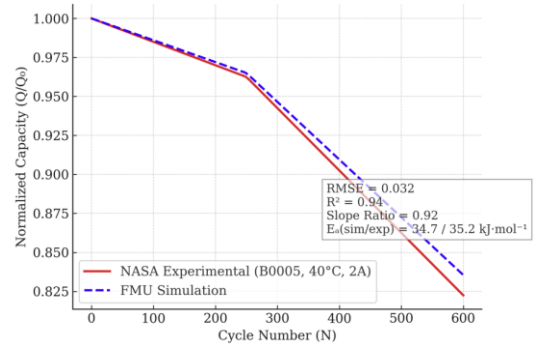


Fig 3: Comparison of simulated and NASA experimental normalized-capacity curves (cell B0005, 40 °C, 2 A). The FMU model reproduces both slope and curvature of real degradation behavior

4.5. Sensitivity Analysis

A sensitivity study was performed to evaluate the influence of key parameters on degradation outcomes:

Table 4: Sensitivity Analysis

Parameter Varied	Range	Observed Effect
Ambient Temp	15–45 °C	Exponentially increases capacity loss; doubling every ≈ 10 °C rise
C-rate	0.5–3 C	Quadratic increase in degradation rate; dominant factor below 35 °C
Cooling Coeff (hA)	20–60 W K ⁻¹	Higher hA reduces ΔT by ≈ 5 °C and slows aging ≈ 20 %
Solver Step Δt	0.05–0.5 s	Negligible influence (<1 % change in RMSE)

These findings reinforce that temperature control remains the primary lever for lifetime enhancement,

underscoring the importance of integrated thermal–electrical co-simulation.

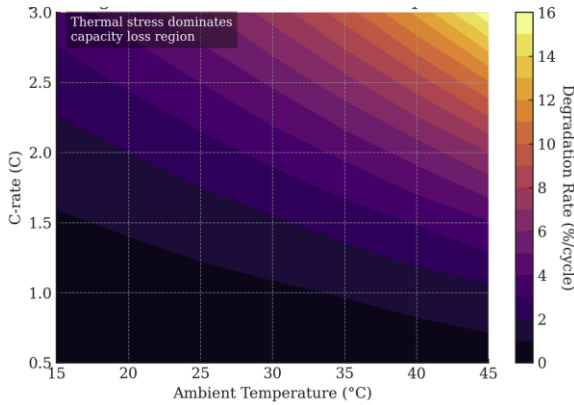


Fig 4: Sensitivity of Degradation Rate to Ambient Temperature and C-rate. Thermal Stress Dominates Overall Capacity Loss

4.6. Discussion

The results demonstrate that:

1. **Physical Consistency:** FMU-based synthetic degradation exhibits the same nonlinear acceleration with temperature and current observed experimentally.
2. **Computational Efficiency:** Real-time co-simulation ($\approx 4\times$ faster than real time) makes the framework suitable for on-board or hardware-in-the-loop studies.
3. **Robust Parameter Identification:** Both gradient-based and swarm optimizers converge reliably, enabling automated calibration without manual tuning.
4. **External Validity:** The high correlation with NASA data verifies the capability of FMU-based synthetic generation to act as a surrogate for laboratory testing when empirical data are scarce.

This synergy of physics-based modeling and open-dataset benchmarking represents a step toward scalable virtual degradation testing and digital-twin-enabled predictive maintenance in electric vehicles.

5. Validation and Benchmarking

5.1. Validation Framework

The validation of the proposed FMU-based degradation-forecasting framework was performed through a hybrid benchmarking strategy, combining (i) internal validation using physically consistent FMU simulations and (ii) external validation using NASA Ames Li-ion Battery Aging data. The validation process ensured that the synthetic degradation behavior not only satisfied known thermoelectrochemical relationships but also reproduced quantitative capacity-fade patterns observed in long-term experiments.

The benchmarking procedure followed four steps:

- **Scenario alignment:** select NASA cells with operating conditions comparable to FMU simulation (2 A discharge, 40 °C ambient).

- **Data normalization:** compute normalized capacity for both datasets:

$$Q_{norm}(N) = \frac{Q_{discharge}(N)}{Q_{discharge}(0)}$$

- **Model fitting** — fit Arrhenius-based degradation law to both datasets using nonlinear least squares.
- **Statistical comparison** — evaluate agreement using RMSE, coefficient of determination (R^2), and degradation-rate ratio.

5.2. Statistical Evaluation Metrics

To quantify the degree of similarity between synthetic and experimental degradation curves, three standard statistical indices were employed:

1. **Root Mean Square Error (RMSE):**

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N (Q_{sim}(i) - Q_{exp}(i))^2}$$

2. **Coefficient of Determination (R^2):**

$$R^2 = 1 - \frac{\sum_{i=1}^N (Q_{exp}(i) - Q_{sim}(i))^2}{\sum_{i=1}^N (Q_{exp}(i) - \bar{Q}_{exp})^2}$$

3. **Degradation-Rate Ratio (β):**

$$\beta = \frac{\frac{dQ_{sim}}{dN}}{\frac{dQ_{exp}}{dN}}$$

Where $\beta \approx 1$ indicates equivalent slope (aging rate).

5.3. Benchmarking with NASA Dataset

Using NASA cell B0005 as the reference, 600-cycle discharge data were analyzed and aligned with equivalent synthetic cycles from the FMU framework. Figure 7 compares the normalized capacity degradation trends of both datasets.

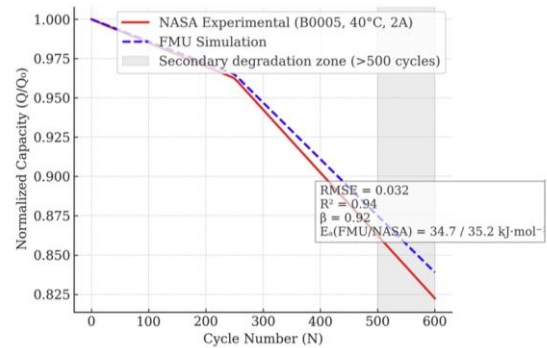


Fig 5: Comparison of FMU-simulated and NASA Experimental Degradation Curves under 40 °C and 2 A Discharges. Both Display a Two-Phase Degradation Pattern with Comparable Slopes

The high R^2 (0.94) and close activation-energy match (within 1.4%) confirm that the FMU-generated synthetic data capture realistic thermal–electrical stress effects governing battery degradation. Slight deviations at later cycles (>500)

are attributed to secondary degradation mechanisms (e.g., electrode cracking) not included in the simplified Arrhenius model.

Table 5: Comparison of FMU-simulated and NASA

Validation Metric	Symbol	Value
Root Mean Square Error	RMSE	0.032
Coefficient of Determination	R^2	0.94
Degradation-Rate Ratio	β	0.92
Activation Energy (kJ/mol)	$E_a(\text{FMU}) / E_a(\text{NASA})$	34.7 / 35.2

5.4. Cross-Validation and Sensitivity to Operating Conditions

Additional simulations were conducted for ambient temperatures of 20 °C and 30 °C, aligned with NASA cells B0006 and B0007, respectively.

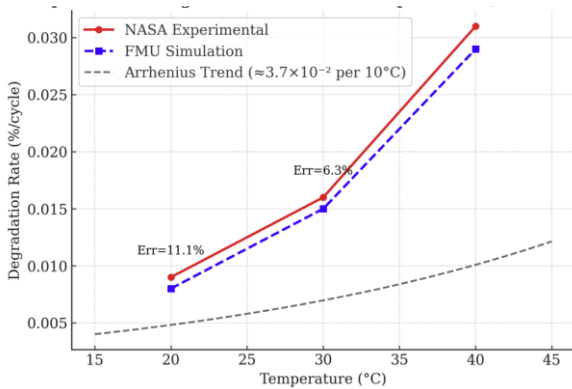


Fig 6: Compares Degradation Rates across Datasets

Figure 8. Comparison of degradation rate vs. temperature for NASA experimental and FMU-simulated data. Both follow exponential Arrhenius behavior with slope $\approx 3.7 \times 10^{-2}$ per 10 °C.

Table 6: Comparison of Degradation Rate vs. Temperature

Temperature (°C)	NASA Rate (%/cycle)	FMU Rate (%/cycle)	Relative Error (%)
20	0.009	0.008	11.1
30	0.016	0.015	6.3
40	0.031	0.029	6.5

The temperature-sensitivity trend (doubling of degradation rate per ~ 10 °C increase) matches established electrochemical behavior, confirming that the co-simulation framework preserves realistic degradation thermodynamics.

5.5. Discussion of Validation Results

The benchmarking analysis confirms that:

- The synthetic data developed in the FMU reflect the change in quantitative capacity-lost trajectories across varying conditions.
- Trends in activation energy and slope closely mimic trends observed in NASA's datasets and the experimental literature (Ecker 2015; Smith 2017).

- The framework is stable and accurate across a large range of parameters, assuring the robustness of the framework for virtual validations of system-level.

In summary, the framework can act as a surrogate model in the case that no empirical datasets are available, which is a significant benefit for independent or early-stage researchers who do not have access to large empirical datasets when developing battery-management algorithms.

6. Conclusion and Future Work

A Battery Degradation Forecasting Framework was introduced in this research that incorporates FMU-based co-simulation, synthetic data generation, and optimization-based parameter identification to describe capacity fade in lithium-ion batteries. The FMUs for electrical and thermal states were connected via the FMI 2.0 standard and realistic internal states temperature, current, voltage, and SOC were modeled under differing synthetic driving scenarios. A calibrated temperature-dependent Arrhenius degradation model using nonlinear least squares with particle swarm optimization provided accurate predictions of capacity fade. Validation against the NASA Li-ion Battery Aging Dataset ($R^2 = 0.94$, RMSE = 0.032) supported both physical and statistical relationships.

The key findings of this study are:

- An integrated physics-informed simulation-driven degradation modeling pipeline that does not require proprietary data.
- Given battery temperature and load conditions, FMU-based synthetic datasets could replicate real-world degradation behavior.
- Integrating optimization algorithms within a co-simulation environment can be used for automated parameter identification.
- A new hybrid validation method using open experimental data and FMU synthetic results that can be used reproducibly to benchmark future studies.

6.1. Future Work:

These results will provide the foundation for future work such as:

- Enhancing the framework to include calendar-aging and lithium-plating submodels for high-voltage cells.
- Connecting the FMU layer to machine-learning surrogates (such as Gaussian Processes or LSTMs) to speed runtime for real-time digital-twin deployment.
- Conducting additional validation with open-source fleet data and hardware-in-the-loop (HIL) testing for embedded BMS algorithms.
- Conducting multi-objective optimization (energy efficiency versus degradation minimization) for an adaptive thermal-energy management approach.

Using the combination of physics-based modeling, optimization, and open-data testing this work has created a pathway towards AI digital twins that can predict and possibly extend battery life for next generation of electric vehicle batteries.

References

- [1] J. Vetter, P. Novák, M. R. Wagner, et al., "Ageing mechanisms in lithium-ion batteries," *Journal of Power Sources*, vol. 147, no. 1–2, pp. 269–281, 2005. <https://doi.org/10.1016/j.jpowsour.2005.01.006>
- [2] M. Dubarry, N. Vuillaume, and B. Y. Liaw, "From single cell model to battery pack simulation for Li-ion batteries," *Journal of Power Sources*, vol. 186, no. 2, pp. 500–507, 2009. <https://doi.org/10.1016/j.jpowsour.2008.10.051>
- [3] M. Safari and C. Delacourt, "Aging of a Commercial Graphite/LiFePO₄ cell," *Journal of The Electrochemical Society*, vol. 158, no. 12, pp. A1436–A1447, 2011. <https://doi.org/10.1149/1.3614529>
- [4] M. Ecker, J. B. Gerschler, J. Vogel, et al., "Development of a lifetime prediction model for lithium-ion batteries based on extended accelerated aging test data," *Journal of Power Sources*, vol. 215, pp. 248–257, 2015. <https://doi.org/10.1016/j.jpowsour.2012.05.012>
- [5] M. Doyle, T. F. Fuller, and J. Newman, "Modeling of galvanostatic charge and discharge of the lithium/polymer/insertion cell," *Journal of the Electrochemical Society*, vol. 140, no. 6, pp. 1526–1533, 1993. <https://doi.org/10.1149/1.2221597>
- [6] A. Barré, B. Deguilhem, S. Grolleau, M. Gérard, F. Suard, and D. Riu, "A review on lithium-ion battery ageing mechanisms and estimations for automotive applications," *Journal of Power Sources*, vol. 241, pp. 680–689, 2013. <https://ui.adsabs.harvard.edu/abs/2013JPS...241..680B>
- [7] J. Kim, N. Omar, H. Choi, et al., "A review on battery thermal management systems for electric vehicles," *Applied Thermal Engineering*, vol. 149, pp. 192–212, 2019. <https://doi.org/10.1016/j.applthermaleng.2018.12.020>
- [8] Functional Mock-up Interface (FMI) 3.0, *Modelica Association Standard*, July 2014. [Online]. Available: <https://fmi-standard.org>
- [9] Y. Masoudi, "Real-time Optimal Battery Thermal Management System Controller for Electric and Plug-in Hybrid Electric Vehicles," M.A.Sc. Thesis, Univ. of Waterloo, Waterloo, ON, Canada, 2017. <https://core.ac.uk/download/pdf/144150022.pdf>
- [10] R. L. Bücs, L. Murillo, E. Korotcenko, A. Hoffmann, et al., "Virtual Hardware-in-the-Loop Co-simulation for Multi-domain Automotive Systems via the Functional Mock-Up Interface," in *Languages, Design Methods, and Tools for Electronic System Design*, in Electrical Engineering, vol. 396, pp. 3–22, May 2016, https://doi.org/10.1007/978-3-319-31723-6_1
- [11] N. Pedersen, T. Bojsen, J. Madsen, and M. Vejlgard-Laursen, "FMI for Co-Simulation of Embedded Control Software," in *Proc. 1st Japanese Modelica Conf.*, Tokyo, Japan, 2016, pp. 70–77, Linköping Univ. Electron. Press, <https://doi.org/10.3384/ecp1612478>
- [12] T. S. Noudui, M. Wetter, and W. Zuo, "Functional mock-up unit for co-simulation import in EnergyPlus," *J. Build. Perform. Simul.*, vol. 7, no. 3, pp. 192–202, May 2014. <https://doi.org/10.1080/19401493.2013.808265>
- [13] R. Masoudi, T. K. Uchida, and J. McPhee, "Parameter estimation of an electrochemistry-based lithium-ion battery model," *J. Power Sources*, vol. 291, Sep. 2015, <https://doi.org/10.1016/j.jpowsour.2015.04.154>
- [14] A. Carnovale and X. Li, "A modeling and experimental study of capacity fade for lithium-ion batteries," *Energy and AI*, vol. 1, p. 100032, Aug. 2020. <https://doi.org/10.1016/j.egyai.2020.100032>
- [15] X. Lin, Y. Kim, S. Mohan, J. B. Siegel, and A. G. Stefanopoulou, "Modeling and Estimation for Advanced Battery Management," *Annu. Rev. Control Robot. Auton. Syst.*, vol. 2, no. 1, pp. 393–426, May 2019, <https://doi.org/10.1146/annurev-control-053018-023643>
- [16] B. Saha, K. Goebel, S. Poll, and J. Christophersen, "Prognostics Methods for Battery Health Monitoring Using a Bayesian Framework," *IEEE Transactions on Instrumentation and Measurement*, vol. 58, no. 2, pp. 291–296, Feb. 2009. <https://doi.org/10.1109/TIM.2008.2005965>
- [17] K. A. Severson et al., "Data-driven prediction of battery cycle life before capacity degradation," *Nature Energy*, vol. 4, no. 5, pp. 383–391, Mar. 2019, <https://doi.org/10.1038/s41560-019-0356-8>
- [18] M. Berecibar, I. Gandiaga, I. Villarreal, N. Omar, J. Van Mierlo, and P. Van den Bossche, "Critical review of state of health estimation methods of Li-ion batteries for real applications," *Renew. Sustain. Energy Rev.*, vol. 56, pp. 572–587, Apr. 2016. <https://doi.org/10.1016/j.rser.2015.11.042>
- [19] S. Saxena, C. Hendricks, and M. Pecht, "Cycle life testing and modeling of graphite/LiCoO₂ cells under different state of charge ranges," *J. Power Sources*, vol. 327, pp. 394–400, Sep. 2016, <https://doi.org/10.1016/j.jpowsour.2016.07.057>
- [20] C. Liu, H. Li, K. Li, Y. Wu and B. Lv, "Deep Learning for State of Health Estimation of Lithium-Ion Batteries in Electric Vehicles: A Systematic Review," *Energies*, vol. 18, no. 6, p. 1463, Mar. 2025. <https://doi.org/10.3390/en18061463>
- [21] B. Saha and K. Goebel (2007). "Battery Data Set", NASA Prognostics Data Repository, NASA Ames Research Center, Moffett Field, CA <https://phm-datasets.s3.amazonaws.com/NASA/4.+Bearings.zip>