A COMPARATIVE ANALYSIS OF BATTERY PERFORMANCE PREDICTION MODELS

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Abstract. Battery modeling is essential for understanding degradation mechanisms, tracking State of Health (SOH), and forecasting Remaining Useful Life (RUL). The article presents a systematic analysis of model classes based on criteria such as accuracy, data requirements, uncertainty, quantification, robustness, computation cost, and interpretability. Key features, limitations, and challenges are summarized for different classes of battery models.

Keywords: battery; models; challenges; performance; characteristics

1. INTRODUCTION

The increasing use of batteries for various applications and various operating conditions has led to increased scientific interest in ensuring their safety, performance, and lifespan. For example, for electric vehicles (EVs) alone, an annual demand for batteries of 5÷8 TWh is predicted in 2040 [1-3]. Although some battery systems on the market qualify as "generation 3", their performance still does not meet the expectations set for 2030 [4].

Battery performance is a key factor in energy storage systems and the efficiency of global applications. Optimizing battery performance is becoming more important than ever with the increasing demands of modern applications and functions. On the other hand, battery modeling is essential not only for predicting battery performance but also for their design and manufacturing.

Battery modeling encompasses a wide spectrum, from empirical and equivalent circuit models, through electrochemical approaches, to advanced statistical methods,

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Machine Learning (ML), and hybrid methods. Determining the accuracy and quantifying the uncertainty (UQ) of the models that act as representations of the actual battery is critical.

There is no clearly presented, implementation-oriented, generalized algorithmic framework for using the different classes of battery models in scientific publications. There are overview publications of the model classes, but they are oriented towards the requirements of certain applications or certain types of batteries. To outline the development trends, taking into account the state-of-the-art of battery model applications, their key characteristics and related advantages and disadvantages, as well as the trends in their improvement, the most significant publications in the field from the last two years have been analyzed [5-21].

Chapter 2 presents simplified flowcharts for each modeling category, the model types for each category, and Recommended Applications.

Chapter 3 presents a comparison of model classes by basic criteria such as Accuracy, Plausibility and Validity, Data requirements, Uncertainty Quantification (UQ), Robustness and Generalizability, Computational requirements, and Interpretability.

Chapter 4 summarizes the future development directions of the next generation of models for the different approaches to battery modeling.

2. BATTERY MODEL CATEGORIES

Accurate prediction of battery performance – including state of health (SOH), capacity fade, internal resistance build-up, and remaining useful life (RUL) – is a specific system task. Battery modeling is essential for understanding degradation mechanisms, tracking State of Health (SOH), and forecasting Remaining Useful Life (RUL).

Predicting the RUL of a battery is the primary approach to ensuring its reliability. A combined graph (SOH + Survival) and PDF/CDF subplot is shown in Fig.1 to obtain an overall prediction of the reliability of a commercial 18650 Li-ion battery under a Weibull model of the survival function (1). The upper figure shows the SOH degradation and survival probability plots, and the lower one shows the PDF and CDF for the remaining life. Both are with the RUL confidence interval colored and the mean highlighted.

$$S(t) = exp(t/\eta)^{\beta} \quad (1)$$

where $S(t)$ – survival function in the Weibull model for survival probability, t – time or cycles, β – shape parameter η – characteristic life.

The estimation SOH and Survival Probability of a battery based on experimental degradation data includes a Modeling Phase. During the modeling phase, three types of models can be used: Deterministic, Probabilistic, or hybrid models. When modeling only SOH, curve-fitting or empirical approaches can be used, which belong to deterministic models. If we model only survival probability, Survival / Weibull / Cox approaches can be used, which are probabilistic models. When simultaneously modeling SOH, the probability of survival with uncertainty bounds, approaches such as the Combination of data-driven degradation mapping and physics-based reliability are used, which are hybrid models.

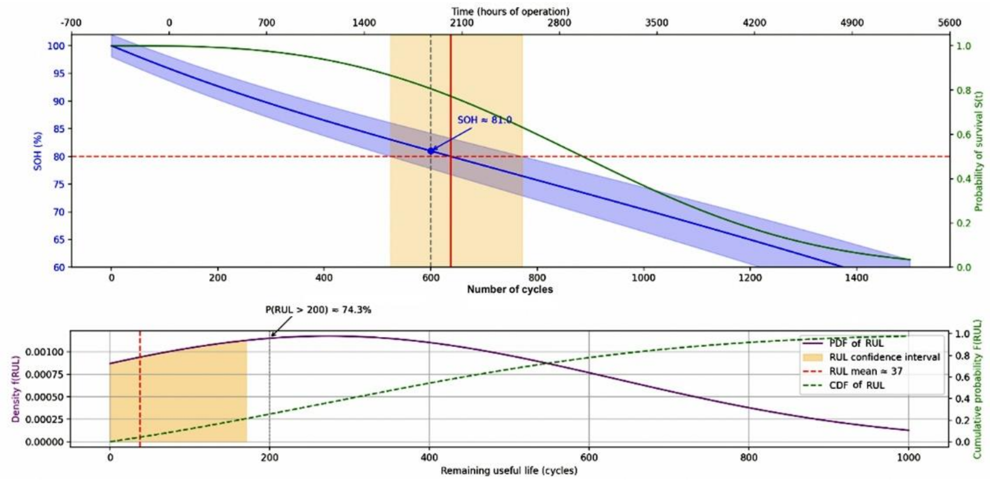

Fig. 1. Reliability assessment – combined visualization: SOH + Survival + PDF/CDF RUL

Battery modeling covers a spectrum of approaches shown in Fig. 2. Each approach represents a different point in the trade-off space among fidelity, generalizability, data requirement, and computational cost.

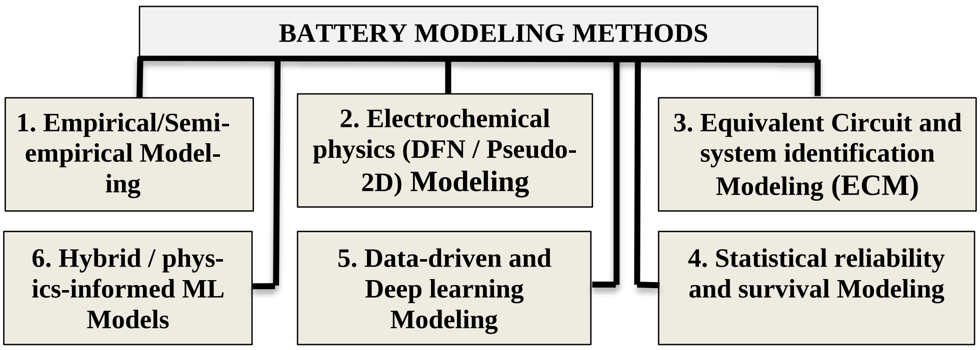

Fig. 2. General classification of battery modeling [5-21]

Simplified flowcharts for each modeling category – from empirical fitting to hybrid physics-informed ML are shown in Fig. 3. Two separate flowcharts are presented to highlight the features of the Data-driven model class when using Machine learning or Deep learning.

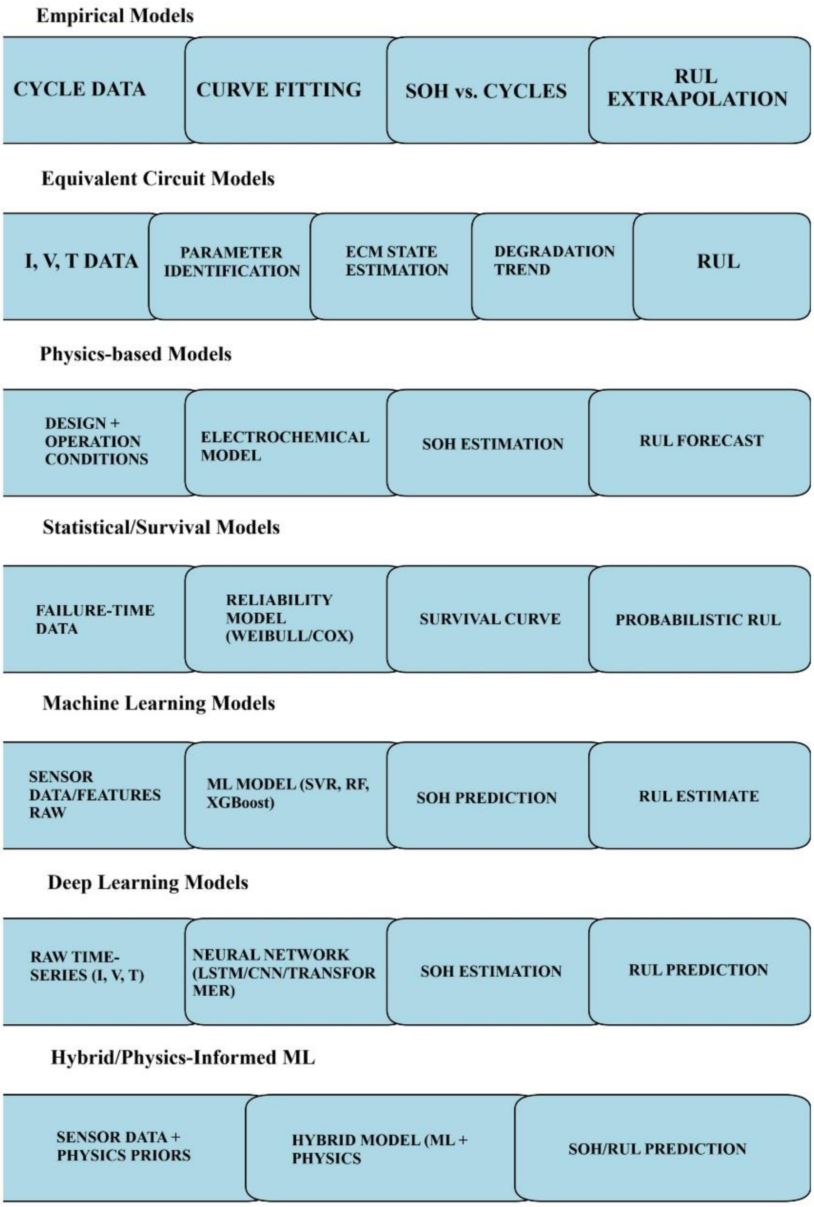

Fig. 3. Simplified flowcharts for each battery modeling category

2.1 Empirical / Semi-empirical models of battery

Empirical models can be categorized according to the mathematical form and the target performance variable as: Polynomial and exponential models, Semi-empirical aging models, Arrhenius-type and Peukert-law formulations, Statistical regression and curve smoothing methods.

Empirical and curve-fitting models are most suitable for:

- Battery management systems (BMS) requiring fast estimation of state-of-charge (SOC) or state-of-health (SOH) under known operating ranges.
- Initial model prototyping or benchmarking, before transitioning to more complex hybrid or physics-based approaches.
- Lifetime and degradation trend analysis, where the objective is to approximate average capacity decay or resistance increase over cycles.
- Data-driven optimization and control, where empirical mappings serve as surrogate models within larger optimization or reinforcement-learning frameworks.

2.2 Electrochemical physics (DFN / Pseudo-2D) models of battery

Electrochemical or physics-based battery models represent the most physically detailed and theoretically grounded class of modeling frameworks. They are derived directly from the governing equations of electrochemistry and transport phenomena, capturing the internal mechanisms of battery cells with high spatial and temporal resolution. Among these, the Doyle–Fuller–Neuman (DFN) and Pseudo–2D (P2D) models form the foundation for modern electrochemical modeling and simulation of battery behavior.

Electrochemical models vary in complexity depending on the degree of physical detail and the assumptions made to simplify the governing equations. The major types include: Full Doyle–Fuller–Newman (DFN) Model, Single Particle Model (SPM), Enhanced Single Particle Model (ESPM), and Thermal and Degradation-Coupled Electrochemical Models.

Electrochemical physics-based models are best suited for research and advanced design applications where accuracy and physical interpretability are critical, including:

- Battery material design and optimization, supporting electrode formulation and electrolyte composition studies.
- Degradation and lifetime prediction, through the integration of SEI growth, lithium plating, and mechanical stress models.
- Thermal and safety simulations, for understanding heat generation and runaway behavior under high loads.
- Model-based control and diagnostics, where reduced-order versions (e.g., SPM or ESPM) are embedded in Battery Management Systems (BMS).

- Digital twins and physics-informed hybrid models, where DFN models serve as the physical core augmented by data-driven components.

2.3 Equivalent Circuit and System Identification (ECM) models of battery

Equivalent Circuit Models (ECMs) represent one of the most widely used and practically efficient categories of battery models. They describe battery dynamics by approximating electrochemical behavior using combinations of electrical circuit elements such as resistors, capacitors, and voltage sources. ECMs aim to reproduce the external voltage–current–time response of a cell while remaining computationally tractable for real-time applications. When combined with system identification techniques, these models can be precisely tuned to match experimental measurements under diverse operating conditions.

ECMs vary in complexity depending on the level of fidelity required and the nature of the application. Common configurations include: Simple resistive models (Rint Model), Thevenin Model, Dual or Multi-RC Models, Fractional-order ECMs, Thermal–electrical coupled ECMs.

A defining feature of ECMs is their reliance on system identification to determine model parameters. This involves fitting the model to experimental voltage–current data using methods such as:

- Least-squares regression, recursive identification, or Kalman filtering for online adaptation.
- Frequency-domain analysis (e.g., Electrochemical Impedance Spectroscopy, EIS) for initial parameter estimation.
- Optimization algorithms (e.g., genetic algorithms, particle swarm optimization) to improve accuracy and robustness under nonlinear conditions.
- ECMs are particularly well-suited for:
- Battery Management Systems (BMS), where real-time estimation of state of charge (SOC), state of health (SOH), and state of power (SOP) is required.
- State estimation algorithms such as the Extended Kalman Filter (EKF) or Unscented Kalman Filter (UKF), which rely on ECMs as the core predictive model.
- Thermal and safety management studies, through coupled electro-thermal modeling.
- System-level control and optimization, where accurate but computationally light models are essential.

2.4 Statistical reliability and survival models of battery

Statistical reliability and survival models form a distinct class of data-driven analytical frameworks designed to quantify the lifetime behavior, reliability, and failure probability of electrochemical energy storage systems. Unlike physics-based or empirical approaches, these models focus on the probabilistic representation of degradation and failure processes, providing insights into the distribution of Remaining Useful Life (RUL) and uncertainty in end-of-life (EOL) predictions. They have become increasingly relevant for fleet-level battery management, warranty analysis, and risk-informed design.

Reliability-based battery models can be broadly categorized into the following groups according to the type of statistical formulation and failure modeling approach: Classical Lifetime Distribution Models, Weibull Distribution, Exponential and Lognormal Distributions, Gamma and Inverse Gaussian Models, Regression-Based Accelerated Lifetime Models (ALM), Stochastic Process Models, Bayesian and Hierarchical Reliability Models, Cox Proportional Hazards Models (PHM), semi-parametric Cox PHM.

For example, the semi-parametric Cox PHM relates the hazard rate (instantaneous failure probability) to a baseline hazard and covariates (e.g., current, temperature, SOC):

$$h(t|x) = h_0(t)exp(\beta^T x) \tag{2}$$

Statistical reliability and survival models are particularly suitable for applications involving lifetime estimation, risk analysis, and reliability management at various levels of the battery ecosystem: End-of-Life (EOL) and Warranty Forecasting, Remaining Useful Life (RUL) Prediction, Reliability-Based Design Optimization (RBDO), Fleet-Level Reliability and Degradation Tracking, Accelerated Testing and Qualification, Integration with PHM Frameworks.

2.5 Data-driven and Deep learning models of battery

Data-driven and deep learning models represent one of the most rapidly evolving classes of battery modeling approaches. Unlike physics-based or equivalent-circuit frameworks, these models derive empirical mappings directly from data rather than relying on explicit physical or chemical equations. Their main objective is to capture complex nonlinear dependencies among voltage, current, temperature, and state-of-health (SOH) indicators to provide accurate predictions of performance, degradation, and remaining useful life (RUL).

Data-driven battery models encompass a spectrum of machine learning (ML) and deep learning (DL) architectures that vary in structure, data requirements, and interpretability. The most widely used categories include: Classical Machine Learning Models (algorithms such as Support Vector Regression (SVR), Random Forests (RF), Extreme Gradient Boosting (XGBoost), and Gaussian Process Regression (GPR)), Neural Network-Based Models (Shallow Networks), Recurrent Neural Networks (RNNs) and Long Short-Term Memory (LSTM) Models, Convolutional Neural Networks (CNNs), Transformer and Attention-Based Models, Autoencoders and

Variational Autoencoders (VAE), Physics-Informed Neural Networks (PINNs) and Hybrid Data-Driven Models.

Data-driven and deep learning approaches are suited for a wide range of predictive tasks across battery research:

- State-of-Health (SOH) and State-of-Charge (SOC) Estimation
- Remaining Useful Life (RUL) Prediction
- Anomaly and Fault Detection
- Thermal and Safety Monitoring
- Fleet-Level Data Analytics
- Hybrid Integration with Physics Models.

2.6 Hybrid / physics-informed ML models of battery

Hybrid and physics-informed machine learning (PIML) models represent an emerging paradigm in battery modeling that bridges the gap between physics-based modeling and data-driven learning. These models aim to combine the interpretability and physical consistency of mechanistic approaches with the flexibility and predictive power of data-driven algorithms. By embedding physical principles or equations within machine learning frameworks, hybrid models can improve accuracy, generalizability, and robustness under diverse operating conditions while reducing data requirements compared to purely empirical approaches.

Hybrid battery modeling frameworks can be broadly categorized according to the degree of physical coupling and the manner in which physics is integrated with data-driven learning. The principal types include: Physics-Guided Data-Driven Models (PG-DDM) (use data-driven algorithms (e.g., neural networks, Gaussian Processes, or regression trees)), Mechanistic–Machine Learning (MML) Coupled Models (for example Coupling an ECM or P2D model with an LSTM network that learns residual dynamics or aging trends), Physics-Informed Neural Networks (PINNs), Grey-Box Models with Embedded Physical Parameters (maintain explicit physical parameterization (e.g., diffusion coefficient, resistance, capacitance) while using ML to estimate or adapt these parameters online), Surrogate or Reduced-Order Physics Models (as Data-driven surrogates (e.g., Gaussian Processes, neural operator networks, or polynomial chaos expansions), are trained to emulate the behavior of computationally expensive physical models)).

Hybrid and physics-informed battery models exhibit several defining features that distinguish them from conventional data-driven or mechanistic approaches. However, hybrid models also present implementation challenges, such as the need for differentiable physical formulations, careful weighting of physics versus data terms in the loss function, and numerical instability during training.

Hybrid and physics-informed ML models are particularly advantageous in applications where both accuracy and physical consistency are essential:

- State and parameter estimation: Real-time estimation of SOC, SOH, and internal temperature using physics-informed LSTM or Kalman filter hybrids.
- Aging and degradation prediction: Modeling SEI layer growth, lithium plating, or impedance rise through PINN-augmented degradation models.
- Digital twin and system monitoring: Developing hybrid digital twins that couple reduced-order electrochemical models with ML-based adaptation.
- Battery design optimization: Accelerating materials and electrode design by training ML surrogates constrained by electrochemical transport equations.
- Model-based control and BMS integration: Providing fast yet physically grounded predictions for advanced battery management and safety monitoring.
- Cross-domain transfer learning: Reusing physics-informed embeddings to generalize across chemistries (e.g., NMC, LFP) and form factors (cell, module, pack).

Despite their advantages, hybrid and physics-informed ML models face specific technical challenges: High implementation complexity, Trade-off between fidelity and speed, data–model inconsistency, Limited availability of high-quality labeled data, and Calibration difficulty.

3. COMPARISON OF BATTERY MODEL CLASSES BY BASIC CRITERIA

Battery SOH and RUL prediction is a multidisciplinary challenge. The most effective strategies combine physics-based modeling to ensure plausibility with data-driven approaches to capture complex, nonlinear dependencies. Critical success factors include data quality and representativeness, uncertainty-aware prediction, validation with run-to-failure experiments, and adaptive recalibration in the field.

A structured comparison table summarizing the trade-offs between different battery modeling approaches for SOH/RUL prediction is shown in Table 1.

Table 1. Comparison by key criteria of battery modeling approaches [5-21]

Model Class	Accuracy	Data Requirements	Uncertainty Quantification (UQ)	Robustness (generalization)	Computational Cost	Interpretability
Empirical / Curve fitting	Low–Medium	Low (few cycles or capacity points)	Limited (confidence intervals only)	Poor (fails under varying profiles)	Very Low (fast)	High (simple forms)

Model Class	Accuracy	Data Requirements	Uncertainty Quantification (UQ)	Robustness (generalization)	Computational Cost	Interpretability
Equivalent Circuit Models (ECM)	Medium	Moderate (voltage/current responses, lab tests)	Via parameter uncertainty	Medium–High (handles varied duty cycles if calibrated)	Low (real-time feasible)	High (parameters = resistance, capacitance)
Electrochemical / Physics-based	High	Medium (cell design, material, thermal parameters)	Sensitivity analysis, stochastic parameterization	High (valid under wide conditions)	High (requires reduction for real-time)	High (physically grounded)
Statistical / Survival (Weibull, Cox, Bayesian)	Medium	Low–Medium (failure-time data)	Natural (probabilistic survival curves)	Medium (population-level more than cell-specific)	Low	Medium (hazard rates interpretable)
Classical ML (SVR, RF, XGBoost)	High (with good features)	High (requires large run-to-failure datasets)	Add-on (ensembles, bootstrapping)	Medium (suffers domain shift)	Low–Medium (fast inference)	Medium (feature importance)
Deep Learning (LSTM, CNN, Transformer)	High–Very High (when data is abundant)	Very High (large, diverse time-series datasets)	Limited unless Bayesian/ensembles used	Medium–Low (risk under unseen profiles)	High (training costly, inference fast)	Low (black-box, unless XAI applied)
Hybrid / Physics-informed ML	High–Very High	Medium–High (physics constraints reduce data needs)	Possible (Bayesian + physics priors)	High (best compromise, adaptable+grounded)	Medium–High	Medium–High (physics improves explainability)

From the data in Table 1, summarized from scientific publications from the last years [6-21], the following general conclusions can be drawn:

- Physics-based models → best for robustness and interpretability, but computationally expensive.
- ML/Deep models → best for accuracy, but require large data sets and careful quantification of uncertainty (UQ).
- Survival models → best for probabilistic reliability assessment, less for individual SOH tracking.
- Hybrid models → most promising for future deployments (accuracy + plausibility + adaptability).

A radar chart comparing the main battery modeling approaches across criteria like accuracy, data needs, uncertainty quantification, robustness, computational cost, and interpretability is shown in Fig. 4.

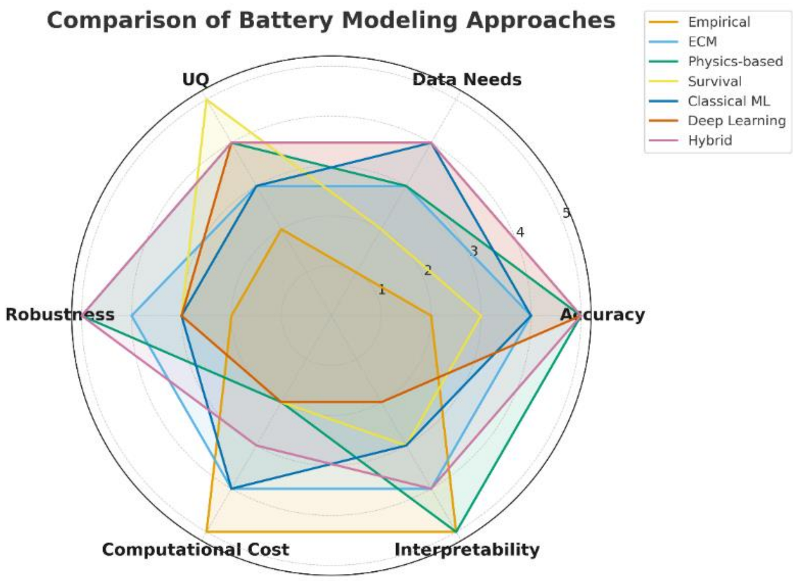

Fig. 4. Radar chart comparing the main battery modeling approaches across different criteria

4. CONCLUSIONS

The study showed that the prospects are in integrating empirical models with machine learning or reduced-order electrochemical elements, forming hybrid empirical-physical models that preserve simplicity while improving predictive robustness.

The development of DFN and P2D models is aimed at using Physics-informed neural networks (PINNs) and surrogate modeling, as well as proper orthogonal decomposition (POD), spectral methods, and lumped-parameter reductions, enabling faster simulation without significant loss of accuracy.

Current research trends focus on hybrid ECM and machine learning frameworks, where neural networks or Gaussian process regressors update ECM parameters in real time, combining interpretability with improved predictive performance.

The perspectives regarding statistical survival models are on their integration with physics-based and machine learning approaches to form hybrid reliability frameworks, combining the interpretability of physical models with the adaptability of statistical learning. Moreover, advances in Bayesian updating, Markov decision processes, and physics-informed survival analysis are extending the role of statistical models in real-time battery health management.

The next generation of data-driven battery models has prospects for the use of Physics-guided deep learning, Federated and continuous learning, Bayesian and probabilistic neural networks, Multi-modal fusion integrating electrical, thermal, and mechanical sensor data streams, and, of course, the application of Lightweight architectures optimized for embedded applications within Battery Management Systems (BMS). Although interpretability and data dependency remain open challenges for data-driven and deep learning models, integration with physically-informed constraints and probabilistic methods promises to further improve their reliability and scientific robustness in next-generation battery management systems.

Emerging research trends aim to further enhance the robustness and generality of hybrid battery models through Differentiable physics solvers, Multiphysics hybridization, Bayesian physics-informed deep learning, Adaptive hybrid digital twins, and Foundation models.

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