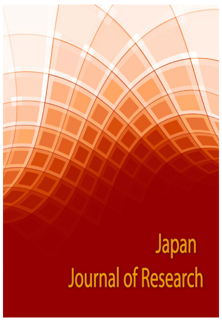
Japan Journal of Research

Original Article



Lithium-Ion Batteries for Electrified Transportation: A Review of Modeling, Degradation, Thermal Management, and Safety

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- Received Date: 11 Jul 2025
- Accepted Date: 20 Jul 2025
- Publication Date: 24 Jul 2025

Keywords

Lithium-ion battery review, battery modeling, battery thermal management, battery aging, electrified vehicles.

Abstract

Lithium-ion batteries (LIBs) have become the cornerstone of modern energy storage, powering applications from consumer electronics to electric vehicles and grid systems. Their high energy density, long cycle life, and reliability have enabled wide-scale adoption. However, challenges related to thermal management, degradation, and safety remain persistent obstacles. This review presents a detailed synthesis of lithium-ion battery technologies, encompassing modeling approaches, thermal behavior, aging mechanisms, and safety concerns such as internal short circuits. Various modeling strategies are examined—electrochemical, mathematical, and equivalent circuit models—that facilitate estimation of internal battery states like State of Charge (SOC) and State of Health (SOH). Temperature's impact on battery performance is analyzed through studies on heat generation, distribution, and management across different operating conditions. Degradation phenomena such as solid electrolyte interphase (SEI) formation and lithium plating are discussed in the context of battery aging, especially for vehicle applications. Additionally, the effects of ambient temperature and battery aging on electric and hybrid vehicle performance are assessed, along with strategies for optimizing battery pack size to enhance fuel economy. By integrating current findings, this review aims to inform future developments in battery design, management, and safety, driving the evolution of LIB technologies toward greater efficiency, durability, and sustainability.

Introduction

Lithium-ion batteries have established themselves as the foundation of modern energy storage technologies, serving an ever-expanding array of applications including smartphones, laptops, electric vehicles (EVs), and large-scale energy storage systems. Their exceptional energy density, long cycle life, and reliable performance under a wide range of operating conditions have solidified their role as the preferred choice for portable and mobile power solutions. However, significant challenges remain, particularly in terms of thermal management, safety, degradation mechanisms, and sensitivity to varying environmental conditions. These limitations continue to motivate a substantial body of research aimed at improving the performance, longevity, and reliability of lithium-ion battery systems.

This review presents a detailed and structured overview of lithium-ion battery technology, encompassing modeling methodologies, thermal and aging behaviors, safety risks—particularly those associated with internal short circuits—and the broader impacts on vehicle performance and battery management. The objective is to synthesize current understanding and trends to guide future research and optimization efforts in the field of lithium-ion battery applications.

Overview of Lithium-Ion Batteries and Their Models

Lithium-ion batteries (LIBs) have become an integral part of daily life, powering a vast range of devices from handheld electronics to full-scale electric vehicles. Over the past three decades, LIBs have evolved from laboratory innovations into a multi-billion-dollar global industry. The remarkable advantages of lithium stem from its electrochemical properties: lithium is the lightest metal and the strongest reducing agent, resulting in a high standard reduction potential. These characteristics translate into batteries that are capable of operating at higher voltages and providing higher gravimetric capacities than most other chemistries.

Among the variations of LIBs, lithium polymer batteries represent a distinct subclass that utilize a semisolid or gel-like polymer electrolyte in place of the traditional liquid electrolyte. These gel polymers offer high ionic conductivity while improving the battery's mechanical stability and resistance to leakage. Depending on the cathode material used, lithium polymer batteries operate across different voltage ranges. For instance, $LiCoO_2$-

Citation: Liu Y. Lithium-Ion Batteries for Electrified Transportation: A Review of Modeling, Degradation, Thermal Management, and Safety. Japan J Res. 2025;6(9):151.

based cells typically function between 2.5 V (fully discharged) and 4.2 V (fully charged), while $LiFePO_4$-based cells operate within 1.8 V to 3.8 V [1,2]. Due to their higher specific energy and better mechanical resilience, lithium polymer batteries are favored in hybrid and electric vehicle (HEV and EV) applications.

Battery performance assessments during charging and discharging cycles require extensive experimentation, often involving highly specialized testing equipment such as cyclers, environmental chambers, data acquisition software, and dedicated computing systems. Given the associated costs and time investment, battery modeling has emerged as a vital alternative, enabling researchers and engineers to predict system behavior and optimize performance without exhaustive physical testing. Modeling is especially crucial for estimating metrics like State of Charge (SOC), State of Health (SOH), and State of Life (SOL), which cannot be directly measured but are essential for monitoring and managing battery usage [3,4].

A variety of battery modeling approaches have been developed, with complexity and fidelity depending on the specific goals—whether for system design, real-time control, or predictive diagnostics [5–23]. These models are broadly categorized into three types: electrochemical models, mathematical or analytical models, and equivalent circuit models [24,25].

Electrochemical models, often considered the most detailed and accurate, simulate the fundamental physical and chemical processes occurring within the battery, including ion diffusion, reaction kinetics, and phase changes. These models are powerful tools for optimizing electrode materials and predicting detailed performance metrics. However, their use is often limited by high computational demands and the need for proprietary parameters, making them more suitable for offline analysis or academic studies [5–8].

Mathematical or analytical models abstract the underlying processes into simplified equations, often derived from curve-fitting experimental data or using semi-empirical relationships. Doyle's foundational model for lithium-ion battery behavior is widely used in this category, offering good computational efficiency but sacrificing some degree of precision [9–12].

Equivalent circuit models represent batteries using lumped electrical components such as resistors, capacitors, and voltage sources. These models approximate battery dynamics and are especially useful for real-time simulation and system-level integration, such as within EV powertrains. They strike a balance between simplicity and accuracy and can account for changes in operating temperature, SOC, and usage patterns [13–23].

Temperature Effects on Lithium-Ion Batteries

The limitations of traditional lead-acid batteries—including high self-discharge rates, large size and weight, and shallow Depth of Discharge (DOD)—have driven the transition toward lithium-ion solutions for automotive and stationary applications. Lithium-ion batteries offer numerous advantages: they are lightweight, compact, exhibit low self-discharge, and support deep DOD without significant performance degradation. Recognizing these benefits, automakers such as Porsche have adopted lithium-ion polymer batteries for Starting, Lighting, and Ignition (SLI) applications [26]. Similarly, many truck manufacturers have transitioned to lithium-based solutions for 12/24 V systems in medium-duty vehicles [27,28].

However, LIBs are not without limitations. One of the most critical performance constraints is their sensitivity to temperature. The operating temperature of a LIB is influenced both by external ambient conditions and internal heat generation during charge and discharge cycles. LIBs generally function effectively between −20 °C and 60 °C [29], with an optimal range of 15 °C to 35 °C [30]. Moreover, it is essential to maintain temperature uniformity across cells in a battery pack, as deviations greater than 5 °C can result in uneven aging, imbalanced performance, and safety risks [30,31].

Temperature extremes impact battery performance differently. At low temperatures, ionic conductivity and lithium-ion diffusion rates decline due to reduced reaction kinetics, leading to lower power output, reduced capacity, and, in extreme conditions, failure to charge [32–34]. Conversely, high temperatures accelerate side reactions, lithium loss, and the degradation of electrode materials, thereby increasing internal resistance and contributing to rapid capacity fade [35]. If unchecked, these effects can trigger thermal runaway, potentially resulting in fire or explosion.

The generation of heat in LIBs arises from multiple mechanisms, including reversible entropy changes, resistive (Joule) heating, and electrochemical reactions [36]. The total heat generation per unit volume, $\dot{q}\left(W/m^3\right)$, is expressed as:

$$\dot{q} = i^2 R + iT\frac{dE_{OC}}{dT}$$

where i (A/m^3) is the volumetric current density, R (Ω) is the internal resistance, T(K) is the temperature, and $dE_{OC}/dT\left(V/K\right)$ is the temperature coefficient of the open-circuit voltage [37]. Notably, studies suggest that Joule heating alone accounts for approximately 54% of total heat generation in many LIB systems [38].

Heat Generation and Temperature Distribution in Lithium-Ion Batteries

Numerous investigations have examined the spatial and temporal distribution of heat generation within LIBs, recognizing its critical role in both performance and safety. One of the pioneering efforts in thermal modeling was presented by Bernardi et al. [39], who proposed an energy balance model incorporating contributions from Joule heat, phase-change heat, heat of mixing, and heat generated during electrochemical reactions. This model assumed a time-dependent but spatially uniform temperature distribution.

Building on Bernardi's framework, Dong and Baek [40] conducted a detailed analysis and determined that under high-rate discharge conditions, irreversible Joule heating was the dominant heat source. In contrast, under low-rate discharge, reversible entropic heat played a more significant role. Similarly, Sato [41] and Lai et al. [42] extended the model by including polarization heat and analyzing thermal behavior as a function of Depth of Discharge (DOD).

Yildiz et al. [43] developed a thermal model specifically for pouch-type LIBs. Their work emphasized the dominance of Joule heating during constant-current discharge and validated the model with empirical data, achieving good agreement across various operating conditions. These studies collectively underscored the importance of accurately characterizing all forms of heat generation to ensure effective thermal management.

Modern computational tools have greatly enhanced the ability to simulate temperature profiles within LIBs. ANSYS Fluent, COMSOL Multiphysics, and MATLAB/Simulink are among the most widely adopted platforms for such modeling tasks.

ANSYS Fluent employs the NTGK (Newman-Tiedemann-Gu-Kim) empirical model, originally introduced by Kwon [44] and later validated by Kim et al. [45,46] with support from Gu's contributions [47]. Samba et al. [48] applied this model to construct a two-dimensional thermal simulation of large-format pouch cells, highlighting the potential for uneven temperature distribution.

COMSOL Multiphysics offers a versatile platform capable of simultaneously simulating electrical, thermal, and chemical processes [49,50]. MATLAB/Simulink provides another valuable toolkit, especially for real-time applications and integrated battery management systems [51]. Wu et al. [52] utilized MATLAB/Simulink to address uneven heat generation in battery modules, providing insights into coupled thermal-electrochemical behavior. Across all models, Joule heating and electrochemical reaction heat remain the principal contributors to battery temperature rise, particularly during fast charging or high-load discharging.

Aging Effects on Lithium-Ion Batteries

Over time, lithium-ion batteries inevitably experience performance degradation due to aging, which manifests as a reduction in both capacity and power capability. This aging process is particularly significant in applications such as electric and hybrid vehicles, where battery longevity directly impacts vehicle utility, resale value, and total cost of ownership [53,54]. The State of Health (SOH) metric is commonly used to quantify battery aging and is typically defined as the ratio of the usable discharge capacity of the aged battery to that of a new cell. Once SOH drops below approximately 80%, the battery is generally considered to have reached its End of Life (EOL) [55].

Post-mortem analysis has played a key role in identifying the root causes of battery aging. Advanced diagnostic techniques such as X-ray diffraction (XRD) [56,57], X-ray photoelectron spectroscopy (XPS) [58], electrochemical impedance spectroscopy (EIS) [59], and scanning electron microscopy (SEM) [60,61] have revealed that two dominant degradation mechanisms are the formation of solid electrolyte interphase (SEI) layers and lithium plating. These processes primarily affect the anode and result in irreversible consumption of active lithium ions, reduced electrode porosity, and increased internal resistance.

The SEI layer forms spontaneously during the first few charge-discharge cycles and continues to evolve throughout the battery's lifespan. While a thin SEI layer can protect the electrode from further degradation, continued thickening of this layer leads to capacity loss. Lithium plating, which occurs when lithium metal is deposited on the anode surface—particularly under high charging rates or low-temperature conditions—poses an even greater risk, as it can eventually lead to internal short circuits [62–65]. Studies show that these passivation layers can grow to hundreds of nanometers over time, severely impeding lithium-ion transport and increasing resistance [66,67]. Recent investigations suggest the SEI consists of a multilayer structure, with a dense inorganic layer adjacent to the anode and a porous organic layer closer to the electrolyte [68–70].

Numerous studies have experimentally analyzed how various operational conditions affect aging. For example, Wang et al. [71] investigated the aging of 18650-type cylindrical cells under 60 different scenarios involving variations in temperature, charge rate, and depth of discharge (DOD). Their results showed that lithium inventory loss was the primary contributor to capacity fade. Similarly, Waldmann et al. [55] conducted aging studies at temperatures ranging from −20 °C to 70 °C, while Schmalstieg et al. [72] validated model predictions against 1C-rate cycle testing of commercial cells. Other researchers, including Atalay et al. [54] and Baghdadi et al. [53], developed aging models incorporating SEI growth and lithium plating, based on extensive cycling data and parametric variation. These studies collectively underscore the multifaceted nature of battery degradation and the importance of carefully controlled operational conditions to mitigate aging.

Internal Short Circuits in Lithium-Ion Batteries

Despite their numerous advantages, lithium-ion batteries are not immune to catastrophic failures, including fire and explosion. Among the most critical hazards is the risk of internal short circuits, which can lead to uncontrolled heating and thermal runaway [73,74]. Battery safety assessments often include abuse tests such as overcharging [75,76], external heating [77,78], mechanical deformation [79,80], and short circuit testing. While external shorts can be mitigated with protective devices like fuses, internal shorts—caused by defects within the cell—are more difficult to detect and prevent [81,82].

Nail penetration testing is a widely used technique to simulate internal short circuits and study their consequences. When a nail punctures a cell, it creates a conductive path between the electrodes, generating intense heat due to the high internal resistance. If the resulting temperature rise is sufficient, thermal runaway may be triggered. This process involves a sequence of exothermic reactions: decomposition of the SEI (~120 °C), electrolyte breakdown (>200 °C), binder decomposition (~240 °C), and cathode material degradation (>250 °C). These reactions release flammable gases, such as carbon monoxide and hydrogen fluoride, which pose further fire and toxicity risks [81–92].

Recent research has focused on visualizing and modeling the dynamics of internal short circuits. Yokoshima et al. [83,84] employed X-ray imaging to observe electrode deformation and gas release during nail penetration in cells of various capacities. Zhao et al. [82] combined experimental tests with numerical simulations to characterize the thermal and electrical behavior under both external and internal short-circuit conditions. Diekmann et al. [85] proposed standardized testing procedures to ensure consistent and reproducible results across different battery formats. Yamanaka et al. [86] developed a combustion risk model tailored for nail penetration scenarios. Furthermore, Feng et al. [81] triggered thermal runaway in a multi-module pack and monitored propagation behavior using embedded sensors to track temperature and voltage shifts. Together, these studies emphasize the critical importance of detecting and mitigating internal short circuits to ensure battery safety.

Ambient Temperature Effects on Electric Vehicles

One of the key obstacles to widespread EV adoption is range anxiety—the concern that a vehicle's battery will not last long enough to complete a journey without frequent recharging. Among the many variables influencing range, ambient temperature plays a particularly significant role. As temperature drops, the internal resistance of lithium-ion cells increases, which reduces power output, limits the maximum allowable charging current, and negatively impacts regenerative braking efficiency [93–96].

Empirical studies have demonstrated the severity of low-temperature effects. For instance, research shows that usable battery capacity declines to approximately 80% when ambient temperature drops from +20 °C to −20 °C, and can fall to as little as 30% at temperatures below −40 °C [94]. A Transport Canada study found that EV driving range at −20 °C was just 45% of the range observed at +20 °C [97], while Hydro Quebec reported an average winter range loss of around 40% compared to summer months [98].

In addition to battery chemistry, auxiliary loads such as climate control systems also influence range. Unlike internal combustion engine (ICE) vehicles that utilize waste heat for cabin warming, BEVs rely solely on battery power to operate heating and cooling systems. This introduces a substantial parasitic load during extreme weather [99]. In cold climates, this can significantly accelerate battery depletion. Kambly and Bradley [100,101] conducted simulations showing that air conditioning (A/C) usage affects BEV range differently depending on geographic location and time of day. Their findings indicate that seasonal range reductions due to HVAC operation can reach up to 23% in hot regions such as Phoenix, Arizona.

Effects of Battery Aging on Electrified Vehicles

Battery aging not only affects the intrinsic properties of lithium-ion cells but also has broader implications for vehicle-level performance. In hybrid electric vehicles (HEVs), the presence of a conventional internal combustion engine alongside the electric drivetrain allows for greater flexibility in power management. This dual-source architecture enables HEVs to strategically manage energy flows, thereby mitigating the impact of battery aging by reducing the reliance on the battery during high-stress conditions [102–104].

Power management algorithms in HEVs are specifically designed to optimize the balance between fuel consumption and battery usage. Several studies have proposed control strategies that factor in the battery's aging state to minimize long-term degradation while still meeting performance demands [103–107]. These strategies include real-time adjustment of power split ratios, optimization of charge-discharge cycles, and intelligent scheduling of energy recuperation.

In contrast, battery electric vehicles (BEVs) rely solely on the electric drivetrain, which places the battery at the center of all propulsion and auxiliary power functions. This dependence heightens the impact of aging, as performance degradation directly influences acceleration, driving range, and charging behavior. In many BEVs, battery management systems (BMS) use pre-defined current, voltage, and temperature lookup tables for cell control [108,109]. However, such static approaches often fail to adapt effectively to evolving battery health conditions.

Advanced cell balancing techniques—both passive and active—are increasingly being explored to manage uneven aging across cells within a battery pack [110]. These methods aim to equalize charge levels and thermal conditions among individual cells to prolong overall pack life. Moreover, the diversity in driver behavior—ranging from aggressive acceleration to prolonged idling—adds complexity to BEV battery management. Consequently, modern BMS development increasingly emphasizes adaptive control strategies that incorporate real-time diagnostics, predictive modeling, and machine learning algorithms to better handle battery degradation without compromising user experience.

Effects of Battery Pack Size on HEV Fuel Economy

In the quest for improved fuel efficiency and reduced emissions, hybrid electric vehicles (HEVs) represent a practical compromise between conventional vehicles and full-electric solutions. Central to their performance is the design and sizing of the onboard battery pack. A battery that is too small limits the vehicle's ability to capture regenerative braking energy and assist in propulsion, while an oversized pack increases system cost, weight, and energy requirements for charging—ultimately reducing fuel economy [111–114].

Optimizing battery pack size involves a trade-off between capacity, cost, weight, and thermal performance. Smaller packs may be insufficient for certain drive cycles, leading to higher fuel consumption and reduced hybrid benefits. Conversely, excessively large packs suffer from diminishing returns in energy savings and may require enhanced thermal management systems to prevent overheating during high-power events.

To address these challenges, researchers have employed a variety of optimization methods. One approach involves multi-objective optimization using algorithms such as particle swarm optimization (PSO) to balance competing goals such as thermal regulation, energy efficiency, and packaging constraints [115]. Other studies have explored model-based methods that simulate daily driving profiles, electricity costs, and thermal load conditions to determine the ideal battery size for specific usage scenarios [116–120]. These efforts underscore the importance of tailoring battery pack design to real-world operating conditions, thereby maximizing fuel economy and minimizing lifecycle costs for HEVs.

Summary

Lithium-ion batteries represent a pivotal technology in the electrification of transportation and the evolution of energy storage systems. Their favorable characteristics—including high energy density, long cycle life, and fast charging capability—have positioned them as the leading choice for applications ranging from portable electronics to electric mobility and grid storage. Yet, the complex interactions among electrochemical, thermal, and mechanical processes pose ongoing challenges.

This review has provided a comprehensive examination of lithium-ion battery technology, spanning modeling techniques, temperature effects, heat generation, and degradation mechanisms. Modeling approaches—whether electrochemical, analytical, or equivalent circuit-based—serve as indispensable tools for estimating internal battery states like SOC, SOH, and SOL. The thermal behavior of batteries, driven by heat generation during operation, significantly influences performance and safety, especially under extreme temperature conditions. Internal short circuits remain a major hazard, with research continuing to focus on detection and prevention. Battery aging, characterized by SEI growth and lithium plating, compromises both capacity and safety, particularly in vehicle applications. Ambient temperature effects, especially in BEVs, impact driving range and efficiency, necessitating sophisticated thermal and power management strategies. Furthermore, battery pack sizing critically affects HEV performance and cost, reinforcing the need for optimized design frameworks.

Overall, continued research and innovation in battery management, thermal regulation, and degradation mitigation are vital to unlocking the full potential of lithium-ion batteries. By addressing the challenges outlined in this review, future generations of energy storage systems can achieve greater efficiency, longevity, and safety, supporting the transition to cleaner and more sustainable technologies.

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