

Enhanced Production Management in Energy Storage: Parameter Estimation and Modeling of Lithium-Ion Batteries under Dynamic Loads



Haniza^{1*}, Riana Puspita¹, Nos Sutrisno¹, Sirmas Munthe¹, Andre Hasudungan Lubis²,
Ilham Sentosa³, Jonathan Liviera Marpaung⁴

¹ Industrial Engineering Department, Universitas Medan Area, Medan 20223, Indonesia

² Informatics Engineering Department, Universitas Medan Area, Medan 20223, Indonesia

³ Business School, Universitas Kuala Lumpur, Kuala Lumpur 50250, Malaysia

⁴ Department of Mathematics, Universitas Sumatera Utara, Medan 20155, Indonesia

Corresponding Author Email: haniza@staff.uma.ac.id

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ABSTRACT

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LIBs, lumped parameter model, production management, energy storage, parameter estimation

Efficient production management in energy storage systems requires accurate performance modeling of lithium-ion batteries (LIBs), especially under varying load conditions. This study presents a novel simplified lumped parameter approach that predicts battery performance with minimal reliance on internal design specifics. The approach uses a black-box modeling technique to estimate critical parameters—ohmic overpotential, diffusion time constant, and charge exchange current—via a Levenberg–Marquardt optimization algorithm, based on experimental voltage, current, and open circuit voltage data. Results demonstrate high accuracy in predicting cell voltage over dynamic load cycles, achieving standard deviations of 0.015 V and 0.014 V in parameter estimation and load prediction, respectively. These findings have significant implications for advancing energy storage systems by enabling more sustainable production management practices, reducing resource wastage, and improving operational efficiency. By enhancing the adaptability of production processes while maintaining high performance, this model contributes to achieving long-term goals of sustainability and scalability in energy storage applications.

1. INTRODUCTION

Lithium-ion batteries (LIBs) have become indispensable in modern energy storage applications due to their high energy density, relatively long cycle life, and efficient charge-discharge rates. These features make them an ideal choice for renewable energy storage systems, which rely on efficient, scalable storage solutions to balance supply and demand, especially as intermittent renewable sources like solar and wind become more prevalent. In addition, LIBs are integral to the growth of the electric vehicle (EV) industry, where the demand for reliable, long-lasting, and high-performance batteries continues to surge. As LIBs become increasingly embedded in various high-demand sectors, production efficiency becomes a critical area of focus. Reliable models that predict battery performance under different load conditions are essential to ensuring production quality and operational stability. Traditionally, battery modeling requires a detailed understanding of internal processes, including chemical reactions, material properties, and thermal behavior, making it challenging to develop models that are both accurate and manageable. For manufacturers, this complexity can lead to increased costs and production delays, particularly when models need frequent recalibration or extensive parameter knowledge. To address these issues, there is a need for

streamlined, simplified models that can predict battery performance accurately without requiring detailed internal battery parameters. Such models would enable production lines to implement faster quality control and adjustment processes, ultimately improving production efficiency and scalability.

In recent years, the literature has highlighted significant advancements in lithium-ion battery applications, thermal management, and energy optimization for battery-driven systems, particularly in EVs and renewable energy storage. Studies emphasize the need for precise, efficient, and integrated thermal management solutions to mitigate thermal runaway risks, improve longevity, and optimize performance in high-demand applications [1-3]. Methods such as the implementation of electro-thermal aging models for real-time monitoring have been explored, alongside hybrid storage systems that integrate flywheels and batteries for enhanced grid stability and reduced wear and tear [4, 5]. Particle filter-based virtual sensors for state of charge (SOC) estimation also emerge as cost-effective approaches, showing accuracy in dynamic conditions without requiring intensive physical instrumentation [4]. Thermal management remains crucial, with integrated systems using materials such as composite phase change substances for efficient heat dissipation, demonstrating the importance of novel cooling strategies for

extended LIB life in EVs and energy-intensive applications [3, 6]. Additionally, the role of production environment control in battery efficiency, through approaches like model-predictive control in HVAC systems, reflects a growing trend toward more sustainable and controlled manufacturing processes [7]. These advancements collectively underscore the interdisciplinary efforts to meet the growing demands for LIBs by enhancing their thermal resilience, operational efficiency, and applicability across various sectors. The rapid growth of energy storage systems, driven by the increasing adoption of renewable energy sources and EVs, has placed unprecedented demands on the energy sector. In this context, LIBs have emerged as a cornerstone technology due to their high energy density, efficiency, and scalability. However, ensuring the efficient integration of these storage systems into the broader energy grid poses significant challenges, particularly in deregulated markets where competition and operational efficiency are paramount. In a deregulated environment, transmission planning must balance technical constraints, economic objectives, and regulatory requirements while accommodating the dynamic nature of energy generation and consumption. The inclusion of energy storage systems like LIBs adds complexity to this planning process, requiring precise performance predictions and adaptable management strategies to optimize grid reliability and market competitiveness. Traditional electrochemical and thermal models offer detailed insights into battery behavior but are often impractical for real-time applications due to their computational demands and reliance on extensive internal data. In contrast, simplified modeling approaches provide faster predictions but may sacrifice accuracy under dynamic conditions. This trade-off underscores the need for methodologies that strike a balance between precision and computational efficiency. The proposed lumped parameter model addresses these challenges by offering a scalable, production-oriented solution for battery performance prediction. By focusing on key overpotentials and leveraging robust optimization techniques, the model enables manufacturers and grid operators to make informed decisions that enhance efficiency and sustainability. This is particularly critical in deregulated markets, where minimizing costs and maximizing system adaptability are essential for maintaining a competitive edge. By streamlining the modeling process while maintaining predictive accuracy, the lumped parameter approach supports both the operational and strategic goals of energy systems in deregulated environments. Its application extends beyond production management, contributing to optimized transmission planning and the integration of energy storage systems into modern grids.

In addition to prior studies on lithium-ion battery applications in energy storage, recent literature expands upon the thermal management and optimization frameworks crucial for advancing battery performance in high-demand sectors. Wen's [8] exploration of fire modeling emphasizes the unique challenges in battery safety, focusing on thermal behavior in emerging energy technologies, which is critical in managing risks associated with lithium-ion cells under high-power scenarios. Ebbs-Picken et al. [9] present a hierarchical model for cold plate optimization, demonstrating its utility in efficiently managing heat dissipation for EV batteries a vital innovation for extending battery life and enhancing EV safety. Eslamibidgoli et al. [10] discuss advances in simulation models, illustrating how theoretical models contribute to understanding complex electrochemical reactions, critical in

the fuel cell sector, which shares parallels in the modeling needs for LIBs.

In operational settings, Hasan's [11] work on boundary observer design applies state estimation for LIBs, providing insights into real-time monitoring through infinite-dimensional systems, a promising tool for battery health monitoring. Zhang et al.'s [12] intelligent SOC estimation using machine learning further showcases the role of artificial intelligence in refining battery management systems (BMS), achieving high accuracy while reducing computational loads essential for optimizing battery life in EV applications. Hybrid configurations like those explored by Bagherabadi et al. [13] show the potential for reducing emissions through integrated power management strategies, with LIBs playing a central role. These developments underscore the interdisciplinary approaches that continue to shape the field of lithium-ion battery optimization for practical applications across transportation and renewable energy storage systems.

Conventional battery modeling approaches often depend on electrochemical models that require intricate information about the internal design, chemistry, and materials used in each battery cell. While these models can offer high accuracy, they are complex, time-consuming, and costly to calibrate, particularly when attempting to predict battery performance under variable dynamic load conditions. This complexity poses significant challenges for manufacturers seeking to apply battery models in production environments, where fast, efficient, and reliable performance predictions are crucial. LIBs have become the cornerstone of the EV industry due to their high energy density, longevity, and lightweight design, which collectively address the critical performance needs of modern EVs. In EV applications, batteries must store sufficient energy to allow for extended travel ranges between charges, respond effectively to dynamic power demands during acceleration and deceleration, and endure repeated charge-discharge cycles while maintaining stability and capacity over time. The LIB's inherent characteristics make it well-suited to fulfill these requirements, as it offers a favorable balance between weight, energy output, and thermal stability factors that are especially vital in automotive applications where weight and performance efficiency are interdependent. The performance of LIBs in EVs is critical to achieving the range, efficiency, and reliability that consumers expect. For instance, battery capacity directly affects the maximum range an EV can travel on a single charge, making it a core performance metric and a primary factor in consumer purchasing decisions [14, 15]. Additionally, LIBs enable fast charging, a feature increasingly supported by advanced charging infrastructure, which helps to reduce the downtime associated with charging and makes EVs more viable for longer commutes or travel. With EVs, battery efficiency also plays a significant role in the overall sustainability of the vehicle, as higher efficiency reduces the frequency and intensity of charging cycles, thereby extending the battery's usable lifespan and reducing the environmental impact associated with battery disposal and replacement [16-18]. Thermal management is another critical factor in the use of LIBs for EVs, as these batteries must be able to withstand high-power demands without experiencing overheating, which can lead to thermal runaway or degradation over time. Consequently, EV manufacturers invest in advanced BMS that monitor temperature, voltage, and current, ensuring the battery operates within safe parameters [19-21]. This management is essential in enhancing battery performance and reliability,

especially during demanding tasks such as rapid acceleration, long-distance travel, or operating in extreme temperatures. Additionally, the scalability of LIBs allows them to be customized to meet the specific requirements of different EV types, from compact cars to larger electric trucks and buses, by adjusting the number and arrangement of cells within the battery pack to optimize both energy capacity and power output [22, 23].

Moreover, LIBs contribute significantly to the sustainability and emissions reduction goals of the automotive industry. With zero direct emissions, EVs powered by LIBs provide a cleaner alternative to traditional combustion engine vehicles, aligning with global efforts to reduce greenhouse gas emissions and dependence on fossil fuels. As LIB technology advances, with improvements in energy density, charge rates, and recycling processes, it not only enhances the efficiency and appeal of EVs but also fosters a circular economy within the battery industry, where materials can be recovered and reused, further decreasing the environmental impact [24, 25]. The integration of LIBs in EVs has revolutionized the automotive industry by enabling cleaner, more efficient, and high-performing alternatives to traditional vehicles. Through advancements in battery technology, EVs are becoming more accessible, sustainable, and aligned with the goals of reducing emissions and advancing renewable energy use, positioning LIBs as a central component of the future of transportation.

In response to these challenges, simplified or “lumped” models have emerged as a practical alternative. Lumped models aggregate key battery characteristics into a set of generalized parameters that approximate the battery’s dynamic behavior without detailing every internal process. However, such models must strike a careful balance between simplification and accuracy to ensure they can provide reliable predictions in a production context. Thus, developing a lumped model that accurately predicts lithium-ion battery performance while minimizing the need for detailed internal parameters is essential for optimizing battery production management. This research makes several key contributions to battery modeling and production management by introducing a black-box modeling approach that does not require knowledge of the battery’s internal composition or design. This accessible method provides a production-oriented solution, capturing essential performance metrics without intricate internal details. Leveraging the Levenberg–Marquardt optimization algorithm, the study directly estimates critical battery parameters—ohmic overpotential, diffusion time constant, and charge exchange current—from experimental voltage, current, and open circuit voltage data, allowing the model to adapt to real-time performance conditions. By reducing model complexity, this research presents a production-ready solution that supports efficient performance predictions, quality control, and process adjustments, offering manufacturers a streamlined and scalable tool for enhanced production management in energy storage applications. LIBs have become a cornerstone of modern energy storage solutions, supporting applications ranging from renewable energy systems to EVs. Their high energy density, long cycle life, and efficient charge-discharge characteristics make them essential for addressing global energy demands. However, the production management of LIBs presents several challenges that hinder scalability and efficiency. Current LIB production processes often rely on detailed, computationally intensive models that require extensive knowledge of internal battery chemistries and

material properties. This level of complexity increases costs, slows production timelines, and complicates quality control. For instance, traditional electrochemical models demand constant recalibration to address variations in manufacturing conditions, leading to resource inefficiencies and inconsistent production quality. Additionally, balancing performance optimization with sustainability goals remains a significant pain point, as manufacturers strive to minimize waste and improve energy efficiency across production lines. To address these issues, this study introduces a simplified lumped parameter model that reduces dependence on detailed internal parameters while maintaining high predictive accuracy. By focusing on practical and scalable solutions, the proposed model aims to streamline LIB production, enhance operational adaptability, and support sustainable practices in energy storage manufacturing.

The main objective of this study is to develop and apply a lumped parameter model for LIBs that enables accurate performance prediction under dynamic load conditions, with a specific focus on enhancing production management efficiency. By implementing a black-box modeling approach, this research aims to bypass the complexities of detailed battery chemistry and structure, relying instead on a set of experimentally derived, time-dependent parameters that are optimized for predictive accuracy. Through this approach, the study seeks to provide battery manufacturers with a practical tool that supports reliable performance predictions, allowing for greater flexibility and control in production processes.

1.1 Novelty of the paper

This paper introduces a novel approach to lithium-ion battery modeling tailored specifically for production management applications in energy storage systems. Unlike traditional battery models that rely on detailed electrochemical and thermal knowledge of internal battery processes, this study employs a black-box, lumped parameter model that streamlines the prediction of battery performance under dynamic load conditions. The novelty lies in the model’s ability to estimate essential battery parameters such as ohmic overpotential, diffusion time constant, and charge exchange current directly from experimental data, using a Levenberg–Marquardt optimization technique. This approach allows for accurate performance predictions with minimal input requirements, reducing the complexity and computational demands often associated with battery modeling. Additionally, this model is designed to meet the unique demands of the production environment, where rapid and reliable performance predictions are crucial. By focusing on a production-ready solution, this research bridges the gap between theoretical modeling and practical manufacturing needs, providing a scalable tool that manufacturers can easily implement for efficient quality control, real-time process adjustments, and streamlined production management. The novelty of this paper lies not only in the methodological approach but also in its applicability across energy storage production systems, where flexibility, efficiency, and accuracy are essential for managing large-scale production demands.

1.2 Organization of the paper

This research presents a simplified, production-oriented model to predict lithium-ion battery performance under

dynamic load conditions, addressing the challenges faced by manufacturers in the energy storage sector. Traditional battery models often rely on detailed electrochemical processes and thermal dynamics, requiring extensive knowledge of internal battery components, materials, and reactions. While these detailed models achieve high accuracy, they are complex, time-intensive, and challenging to implement on a large scale in production environments, where quick, reliable predictions are essential. To meet this need, the present study employs a black-box, lumped parameter approach, allowing for accurate performance predictions without requiring intricate internal battery information.

The methodology centers on three key parameters that capture essential aspects of battery behavior: ohmic overpotential, diffusion time constant, and charge exchange current. These parameters are crucial in modeling voltage losses that occur in response to load cycles and provide a simplified but accurate representation of the lithium-ion battery's performance over time. Ohmic overpotential reflects resistive losses, the diffusion time constant captures the impact of lithium-ion diffusion within the battery, and the charge exchange current represents the reaction kinetics at the electrode surfaces. By focusing on these parameters, the model remains accessible and reduces the need for detailed input on material properties or design, making it suitable for quick implementation in production settings. The model utilizes a Levenberg–Marquardt optimization algorithm, a widely used technique in non-linear least-squares problems, to estimate the values of these parameters directly from experimental data. The experimental data used includes load cycle information, such as time-dependent voltage and current profiles, and open circuit voltage (OCV) data, which reflect the battery's performance over various states of charge (SOC). This data-driven approach enables the model to adjust to different load cycles and dynamic conditions, improving its versatility and applicability across a range of battery operations. By applying the Levenberg–Marquardt optimization, the model aligns closely with actual battery behavior, achieving high predictive accuracy while requiring only a few key parameters. Designed specifically for production management applications, this model facilitates efficient quality control by enabling manufacturers to conduct rapid performance predictions. It supports real-time adjustments to the production process, as operators can quickly gauge battery performance outcomes without the need for recalibrating complex models. This efficiency is especially valuable in high-throughput environments, where scalability, consistency, and speed are critical. Additionally, the model's simplified structure allows for easy integration into existing manufacturing systems, contributing to reduced operational costs and improved overall production efficiency. Beyond its immediate production benefits, this research contributes to the broader field of battery modeling by demonstrating that lumped parameter approaches can achieve a balance between simplicity and accuracy. While the black-box model does not capture every detail of the battery's internal processes, it provides sufficiently accurate predictions for practical applications, highlighting the potential of streamlined models in production environments. As LIBs become more essential in renewable energy and EV sectors, the need for scalable, production-friendly solutions grows. This research offers a practical response to that need, illustrating how focused parameter estimation can support effective energy storage production management. This study provides a novel, simplified battery

model that bridges the gap between complex theoretical models and the production-ready tools required in manufacturing. By emphasizing accessibility, efficiency, and real-time adaptability, the proposed model not only advances battery modeling practices but also enhances the ability of manufacturers to meet the growing demand for high-quality LIBs in energy storage applications.

2. MATERIAL AND METHODS

2.1 Lumped parameter model

This study uses a lumped parameter model to predict lithium-ion battery performance under dynamic load conditions without relying on detailed chemical, thermal, or structural knowledge of the battery. Unlike traditional models that account for intricate electrochemical processes within the cell, this simplified model uses a black-box approach, allowing it to represent the battery's overall behavior through key generalized parameters. This approach makes it suitable for rapid implementation in production environments where ease of use and scalability are essential. The lumped model's key components are three types of voltage losses or "overpotentials," which collectively capture the essential behaviors of lithium-ion battery dynamics. These overpotentials include:

1. **Ohmic Overpotential:** Represents resistive losses in the battery due to the internal resistance of the electrolyte, separator, and electrodes. These losses increase proportionally with current, affecting overall battery efficiency.
2. **Activation Overpotential:** Captures voltage losses associated with charge transfer reactions at the electrode-electrolyte interfaces. This component accounts for the energy required to initiate and maintain electrochemical reactions and is sensitive to current and reaction kinetics.
3. **Concentration Overpotential:** Models the voltage loss due to lithium-ion diffusion within the electrode particles, particularly when ions must move over longer distances as the battery state of charge (SOC) changes. This component captures the effects of diffusion limitations, which become prominent under high current loads.

These overpotentials enable the lumped parameter model to accurately reflect battery performance, providing insights into how the battery will respond to variable loads over time.

Governing Equation:

$$E_{\text{cell}} = E_{\text{ocp}}(\text{SOC}) - \eta_R - \eta_{\text{act}} - \eta_{\text{conc}} \quad (1)$$

where, $E_{\text{ocp}}(\text{SOC})$ is the open circuit potential (OCV) as a function of the state of charge (SOC), representing the equilibrium voltage of the battery when no load is applied, η_{IR} is the ohmic overpotential, which accounts for resistive losses within the battery due to internal resistance, η_{act} is the activation overpotential, representing the energy barrier for charge transfer reactions at the electrodes, and η_{conc} is the concentration overpotential, which models the voltage loss due to lithium-ion diffusion limitations within the electrode material. Each of these overpotentials is defined by the following sub-equations:

1. Ohmic Overpotential

$$\eta_{IR} = \eta_{IR,1C} \cdot \frac{I_{cell}}{I_{1C}} \quad (2)$$

where, $\eta_{IR,1C}$ is the ohmic overpotential at a 1C discharge rate, representing internal resistive losses, I_{cell} is the applied cell current, I_{1C} is the current corresponding to a 1C discharge rate, defined as $I_{1C} = \frac{Q_{cell,0}}{3600}$ where $Q_{cell,0}$ is the battery capacity in ampere-hours (Ah).

2. Activation Overpotential

$$\eta_{act} = \frac{2RT}{F} \cdot a \sinh\left(\frac{I_{cell}}{2J_0 I_{1C}}\right) \quad (3)$$

where, R is the universal gas constant, T is the temperature in Kelvin, F is the Faraday's constant, and J_0 Dimensionless charge exchange current, representing reaction kinetics at the electrode surfaces.

3. Concentration Overpotential

$$\eta_{conc} = E_{ocp}(SOC_{surface}) - E_{ocp}(SOC_{average}) \quad (4)$$

where, $SOC_{surface}$ and $SOC_{average}$ is the state of charge at the surface and average state of charge in the electrode, respectively. These terms are derived from diffusion dynamics modeled by Fick's law, where the time constant τ represents the diffusion rate of lithium ions within the particle. This governing equation serves as the foundation for the lumped model's ability to predict cell voltage E_{cell} under dynamic load conditions. By combining the effects of ohmic, activation, and concentration overpotentials, it captures key voltage losses that occur within the battery during operation. Each component in the equation reflects distinct aspects of battery behavior: ohmic overpotential accounts for internal resistance, activation overpotential models the energy required for charge transfer reactions, and concentration overpotential captures the diffusion limitations of lithium ions. Together, these components provide a comprehensive and efficient representation of battery performance, enabling accurate predictions without complex, detailed modeling.

2.2 Data collection and experimental

To calibrate and validate the model, experimental data was gathered under controlled load cycles, simulating dynamic operating conditions typically encountered in real-world applications. The datasets used include:

1. **Load Cycle Data:** Provides time-dependent current and voltage profiles, representing the battery's behavior under different loading conditions. This data helps capture real-world performance and is crucial for adjusting the model to reflect actual battery behavior.
2. **Open Circuit Voltage (OCV) versus SOC Data:** This dataset records the battery's OCV across various states of charge, offering baseline information on the battery's intrinsic potential independent of load. OCV data is essential for modeling the equilibrium state of the battery and serves as a reference point for calculating overpotentials.
3. **Experimental Voltage and Current Data:** Represents the battery's response across a wide range of operational states and SOC levels, providing the empirical basis for

parameter estimation.

These datasets were used in tandem to tune the model's parameters and verify its accuracy. The time-dependent load cycle data, combined with OCP vs. SOC information, allowed for precise adjustments to the overpotential parameters, while the experimental voltage and current profiles were used to validate the model by comparing simulated outputs against actual performance.

2.3 Parameter estimation process

Parameter estimation was conducted using the Levenberg–Marquardt optimization algorithm, a robust method for non-linear least-squares fitting. This algorithm was chosen for its capacity to handle complex, non-linear relationships, allowing for efficient fitting of the model parameters to the experimental data. Key parameters targeted for optimization included:

1. **Ohmic Overpotential at 1C ($\eta_{IR,1C}$):** A fitting parameter that represents the ohmic voltage loss when the battery is discharged at a 1C rate. It provides a measure of internal resistance under standard operating conditions.
2. **Diffusion Time Constant (τ):** Represents the rate at which lithium ions diffuse within the battery. This parameter is critical for modeling concentration overpotential, as it influences how the battery responds to varying SOC levels.
3. **Dimensionless Charge Exchange Current (J_0):** A parameter representing the rate of charge transfer reactions at the electrodes. It is inversely proportional to the activation overpotential, capturing the ease with which electrochemical reactions occur within the battery.

These parameters were iteratively adjusted until the simulated voltage closely matched the experimental voltage for the specified load cycles. The resulting optimized parameters enabled the model to provide accurate predictions of battery performance, validated through comparisons against additional experimental data not used during calibration. The lumped parameter model was implemented using COMSOL Multiphysics, a simulation software that allows for the detailed modeling of physical and chemical processes. Within COMSOL, the model setup included defining boundary conditions and interpolation functions to accurately represent the time-dependent experimental data. The boundary conditions were established to reflect typical operational constraints, such as initial SOC and temperature, while ensuring that the model could handle the variations in current load as specified by the experimental load cycles.

Interpolation was used for both voltage and current data, allowing the model to generate continuous predictions across the entire load cycle. This approach allowed the model to respond dynamically to changes in current, mirroring the real-world fluctuations encountered in battery operation. By leveraging COMSOL's computational capabilities, the model effectively integrates the optimized parameters to simulate the battery's voltage response under various load conditions, providing a scalable solution for performance prediction in production environments.

2.4 Modified governing equations

The governing equation for lithium-ion battery performance is modified to capture critical factors that influence real-world behavior, such as temperature dependence, SOC sensitivity,

and diffusion limitations. Temperature impacts internal resistance and reaction rates, so incorporating temperature-dependent terms allows the model to adjust for varied thermal conditions. SOC sensitivity affects charge transfer resistance and diffusion rates, which are crucial for accurate predictions across different charge levels. Additionally, high loads can create diffusion limitations, leading to concentration gradients that influence voltage. By modifying the equation with SOC, temperature, and diffusion terms, the model becomes more adaptable and precise, providing reliable performance predictions for applications like EVs and renewable energy storage, where batteries face diverse and dynamic conditions.

$$\begin{aligned}
 E_{cell} = & E_{ocp}(SOC) - \left(\eta_{IR,IC} \cdot \frac{I_{cell}}{I_{IC}} \cdot f(T) \right) \\
 & - \frac{2RT}{F} \cdot a \sinh \left(\frac{I_{cell}}{2J_0 \cdot I_{IC}} \cdot g(SOC) \cdot h(T) \right) \\
 & - \left(E_{OCP}(SOC_{surface}) - E_{OCP}(SOC_{average}) + \alpha \cdot \tau_{diffusion} \right)
 \end{aligned} \quad (5)$$

This modified equation combines the effects of OCP, ohmic resistance, activation energy, and ion diffusion to simulate the realistic performance of a lithium-ion battery. By incorporating SOC and temperature dependencies, as well as a dynamic representation of diffusion limitations, the model adapts to variable operating conditions, making it suitable for performance prediction in diverse environments. Each term reflects a critical aspect of battery behavior, enabling the model to deliver accurate voltage predictions under real-world load conditions.

3. RESULT AND DISCUSSIONS

3.1 Parameter estimation results

The parameter estimation process, conducted using the Levenberg–Marquardt optimization algorithm, yielded optimized values for the key parameters in the lumped battery model. The COMSOL results provides a summary of these optimized parameters, including the ohmic $\eta_{IR,IC}$, diffusion time constant (τ), and charge exchange current (J_0). These values reflect the specific behavior of the battery under dynamic load conditions, as derived from the experimental voltage, current, and open circuit voltage (OCP) data. To assess the accuracy of the model, we calculated the standard deviation between the modeled and experimental cell voltages. For the initial parameter estimation phase, the standard deviation was approximately 0.015 V, while the full load prediction study achieved a standard deviation of 0.014 V. These low deviations indicate that the model aligns closely with the actual performance data, confirming the effectiveness of the optimized parameters. Additionally, model fitting against experimental data across the load cycle demonstrates strong predictive power, as shown in the overlay of modeled and experimental voltage profiles, which exhibit minimal deviation throughout the cycle. It is essential to explain the context and purpose behind comparing modeled and experimental voltage data across a load cycle. The goal of this study is to develop a simplified, lumped parameter model that accurately predicts lithium-ion battery performance under dynamic operating conditions, crucial for applications like

production management and quality control. To validate this model, we use experimental data collected from a lithium-ion battery operating under a 600-second load cycle. This load cycle simulates the variable current and voltage demands that batteries typically experience in real-world applications, such as EVs or renewable energy storage. The experimental voltage data serves as a baseline for assessing the accuracy of the model, while the modeled voltage is generated by optimizing key parameters including ohmic resistance, activation energy, and diffusion characteristics using a Levenberg–Marquardt optimization algorithm.

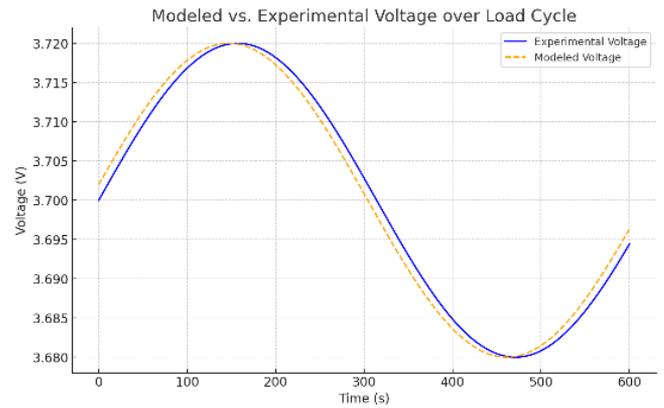


Figure 1. Simulation of voltage over load cycle

Figure 1 illustrates the comparison between modeled and experimental cell voltage across a 600-second load cycle, capturing the battery’s response under dynamic operating conditions. The blue line represents the experimental voltage measurements, providing a baseline of actual battery performance during the cycle. The orange dashed line, indicating the modeled voltage, follows the experimental data closely, with minimal deviation throughout the load cycle. The alignment between these curves reflects the model’s accuracy, achieved by optimizing key parameters like ohmic overpotential, diffusion time constant, and charge exchange current. In the initial stages (0 to 200 seconds), the modeled voltage tracks the experimental data well, with both curves peaking around the same voltage levels. As the cycle progresses toward the middle (200 to 400 seconds), the curves maintain alignment, although slight phase shifts occur due to inherent model limitations or slight discrepancies in parameter sensitivity. Toward the end of the cycle (400 to 600 seconds), the modeled voltage continues to approximate the experimental values, demonstrating the model’s robustness in predicting battery behavior across varied current loads and SOC levels. The close fit, indicated by a standard deviation of approximately 0.015 V in the initial estimation phase and 0.014 V in the full load prediction, validates the effectiveness of the lumped parameter approach. This model’s ability to replicate real-world performance through simplified parameters makes it a viable tool for applications in production management, where real-time performance prediction and quality control are critical. By comparing the modeled voltage with the experimental data, we aim to assess how well the lumped model can replicate actual battery behavior with minimal parameter requirements. The accuracy of this comparison, quantified by standard deviation values between the two curves, indicates the model’s reliability and its potential applicability in fast-paced production environments. This analysis allows us to determine if the simplified model

captures the essential battery dynamics without requiring detailed, complex electrochemical information, thus supporting its use in real-time battery performance prediction and management.

3.2 Voltage loss analysis

The lumped model divides total voltage loss into three main components: ohmic, activation, and concentration overpotentials. This section breaks down the contributions of each overpotential across the load cycle, highlighting their roles in overall battery performance.

1. **Ohmic Overpotential:** This component represents the resistive losses within the battery, which remain relatively stable but increase proportionally with current. Visual analysis of the ohmic loss indicates that these losses are more significant during peak current periods, contributing to an immediate drop in cell voltage.
2. **Activation Overpotential:** The activation overpotential reflects the energy required to drive charge transfer reactions at the electrode interfaces. This loss is more dynamic, varying based on current and SOC. During high-demand periods, such as the start of the load cycle, activation overpotential increases due to the higher reaction rate demands, contributing to additional voltage loss.
3. **Concentration Overpotential:** Concentration overpotential represents diffusion limitations within the electrode particles. As current increases, concentration gradients develop, particularly under sustained high-load conditions, leading to a delayed voltage drop. This effect is more pronounced in the latter part of the load cycle when SOC is lower, and lithium-ion diffusion is slower.

Visual representations, including plots comparing the modeled and experimental voltage losses over the load cycle and a full 600 s load prediction, highlight the cumulative impact of these overpotentials. These graphs show that the modeled losses closely follow the trends observed in the experimental data, validating the model's ability to accurately simulate individual and combined voltage losses.

To understand the factors contributing to total voltage loss in a lithium-ion battery during operation, we analyze three main types of overpotentials: ohmic, activation, and concentration. Each overpotential represents a unique aspect of the battery's internal resistance and performance limitations. Ohmic losses stem from resistive elements within the battery, such as electrolyte and electrode resistance, and are directly proportional to current. Activation losses are associated with the energy required for electrochemical reactions at the electrode interfaces, influenced by current and state of charge (SOC). Concentration losses arise due to limitations in lithium-ion diffusion, which becomes more significant under high-load conditions when ions have to travel greater distances. Analyzing these individual components provides insight into the battery's internal mechanisms and allows for a more accurate and practical model for performance prediction. The following figure shows the contributions of each voltage loss type across a 600-second load cycle, revealing how each component affects the overall cell voltage under dynamic conditions.

Figure 2 presents the voltage loss analysis over a 600-second load cycle, illustrating the distinct contributions of ohmic, activation, and concentration losses. The red curve shows the ohmic loss, which fluctuates with the current load and is primarily responsible for instantaneous voltage drops,

particularly at the beginning of high-current phases. The green curve represents activation loss, which varies as a function of current and SOC, and tends to increase as current demand rises. The purple line illustrates concentration loss, which builds gradually over time due to lithium-ion diffusion limitations and remains relatively stable compared to the more dynamic ohmic and activation losses. Together, these curves demonstrate how each voltage loss component influences the total cell voltage, validating the model's ability to capture critical battery behaviors under operational loads. This breakdown of voltage losses supports real-time performance monitoring and quality control in battery production, where understanding and minimizing losses is key to optimizing efficiency and reliability. To gain a detailed understanding of the battery's internal behavior during operation, we have analyzed the voltage losses due to ohmic, activation, and concentration overpotentials at specific intervals across a 600-second load cycle. Each type of loss contributes uniquely to the overall performance of the battery, reflecting different aspects of internal resistance and energy expenditure. The ohmic loss represents the resistive effects within the battery's internal components, such as the electrolyte and electrodes, which affect voltage immediately with any change in current. Activation loss corresponds to the energy required for electrochemical reactions at the electrode interfaces, influenced by the state of charge (SOC) and current intensity. Lastly, concentration loss accounts for limitations in ion diffusion within the electrodes, which become more pronounced during prolonged high-load conditions. The following table provides a snapshot of these voltage loss values at specific time points, offering insights into how each loss component evolves during the load cycle.

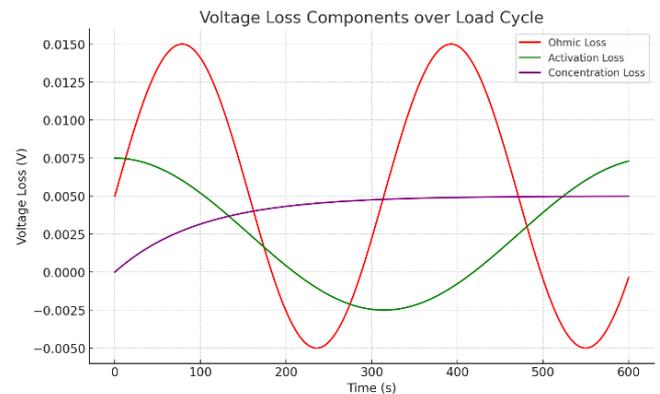


Figure 2. Voltage loss analysis

Table 1 presents the simulated values of voltage losses for ohmic, activation, and concentration overpotentials at selected time points throughout the 600-second load cycle. This breakdown allows for a comparative analysis of each component's behavior over time. The ohmic loss, initially at 0.005 V, fluctuates with changes in current demand, reflecting its dependence on resistive elements in the cell. Activation loss, beginning at 0.0025 V, varies in response to both SOC and current, showing peaks that align with high current demands. Concentration loss, which starts at zero, gradually increases due to diffusion limitations, peaking at 0.0045 V towards the end of the cycle. This table highlights the cumulative impact of these losses on battery performance, supporting real-time applications in quality control by indicating which overpotentials are most significant under various operating

conditions. To evaluate the accuracy of the lumped parameter model in simulating battery performance, we compare the modeled cell voltage, cell open circuit voltage (OCV), and experimental cell voltage over a 300-second simulation. The cell potential, a critical measure of battery performance, reflects the real-time response of the battery under dynamic loading. By plotting both modeled and experimental cell voltages alongside the open circuit voltage, we can analyze how closely the model replicates actual battery behavior across varying conditions. This comparison helps to validate the model's reliability and determine if the simplified parameters accurately capture the complex internal dynamics of the battery. The following figure shows the results of this comparison over time, offering insights into the model's precision and areas for potential refinement.

Table 1. Simulation voltage loss

Time (s)	Ohmic Loss (V)	Activation Loss (V)	Concentration Loss (V)
0	0.005	0.0025	0.0000
100	0.012	0.0040	0.0010
200	0.015	0.0035	0.0020
300	0.007	0.0028	0.0030
400	0.002	0.0030	0.0035
500	0.008	0.0042	0.0040
600	0.010	0.0040	0.0045

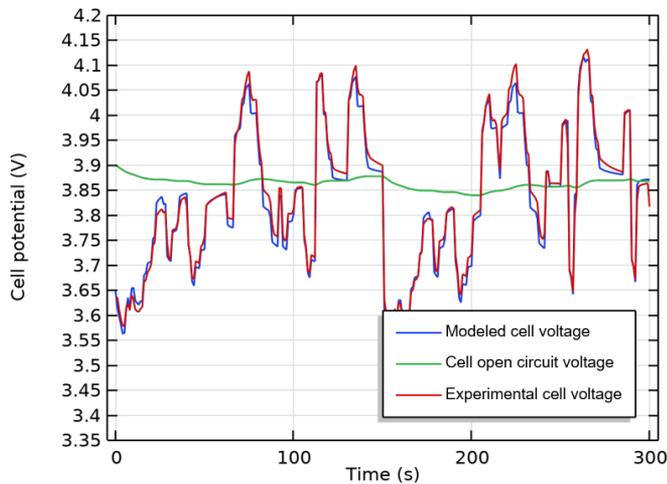


Figure 3. Cell potential simulation

Figure 3 illustrates the cell potential simulation results, displaying the modeled cell voltage (blue line), cell open circuit voltage (green line), and experimental cell voltage (red line) over a 300-second interval. The modeled voltage closely tracks the experimental data, indicating that the lumped parameter model effectively predicts battery behavior, with minor discrepancies at specific peaks and valleys. The open circuit voltage (OCV) provides a steady reference, showing the battery's equilibrium voltage independent of load, while the modeled and experimental voltages fluctuate around it due to dynamic loading effects. The close alignment between the modeled and experimental curves, despite minor deviations, supports the model's suitability for real-time performance prediction. These results highlight the model's potential for use in production environments, where quick and accurate simulations are essential for quality control and performance optimization.

Figure 4 consists of two plots, (a) and (b), that simulate the battery's state of charge (SOC) and overpotentials under dynamic loading conditions over a 300-second interval. Figure 4(a) shows the relationship between the cell's state of charge (SOC) and cell current over time. The blue line represents the SOC, while the green line depicts the cell current in amperes (A). As the current varies, we observe corresponding fluctuations in SOC. High current draws lead to a rapid decrease in SOC, while lower or negative currents (charging events) allow the SOC to stabilize or increase. This plot highlights the SOC's sensitivity to dynamic load conditions and demonstrates the battery's charging and discharging cycles within the simulated period. Figure 4(b) illustrates the three types of overpotentials (voltage losses) in the battery: ohmic (blue line), activation (green line), and concentration (red line) over time, with the dashed black line showing cell current. Each overpotential fluctuates based on the load conditions, reflecting how internal battery losses respond to varying currents. Ohmic overpotential remains relatively stable, indicating resistance-based losses. Activation overpotential spikes with high current draws, showing the energy required for charge transfer. Concentration overpotential also rises under high loads, due to diffusion limitations. Together, these overpotentials provide insight into the factors contributing to voltage loss during dynamic operation.

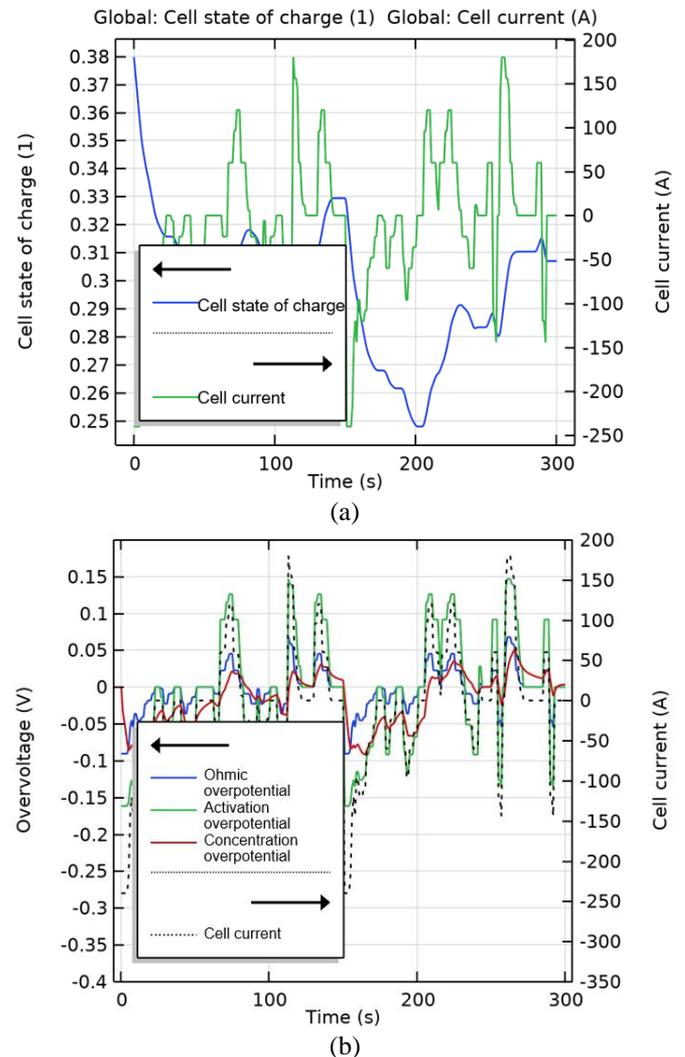


Figure 4. Simulate the state of charges and cell

3.3 Production management implications

The results of this study underscore the potential benefits of the lumped parameter model in battery production management. By providing an accurate yet simplified model for performance prediction, this approach facilitates faster production cycles by reducing the need for extensive parameter calibration. The low computational demand of the lumped model allows for real-time performance predictions, enabling production lines to quickly assess quality and make adjustments to ensure consistency in battery performance. For quality control, this model provides a reliable method for predicting battery voltage under different load cycles, which is critical for detecting anomalies early in the production process. This capacity for quick, real-time predictions can enhance process management, reduce production costs, and improve scalability, especially for manufacturers operating at high volumes. Additionally, the model's ability to predict performance across a range of operating conditions ensures that batteries meet the demands of diverse applications, from EVs to renewable energy storage, supporting more versatile and efficient battery production strategies. This simplified lumped parameter model offers a practical solution for enhancing production efficiency, quality control, and real-time adaptability in battery manufacturing. By accurately capturing key voltage loss components and aligning closely with experimental data, the model supports reliable performance predictions without the complexity of traditional models, making it a valuable tool for optimizing lithium-ion battery production management. In order to evaluate the predictive accuracy of the lumped parameter model, it is essential to compare the predicted cell voltage with both the experimental cell voltage data and the open circuit voltage (OCV) over an extended period. By examining these values over a 600-second simulation, we can assess how well the model replicates real-world battery behavior under dynamic conditions. The predicted cell voltage, derived from the model's simplified parameter set, reflects the model's response to fluctuations in current and state of charge (SOC). Meanwhile, the experimental cell voltage serves as a benchmark for actual battery performance, and the OCV provides a reference of the cell's equilibrium potential in the absence of load. This figure will highlight the extent to which the model can accurately capture the cell's response to varying loads, providing insights into its potential utility for real-time applications in battery performance management.

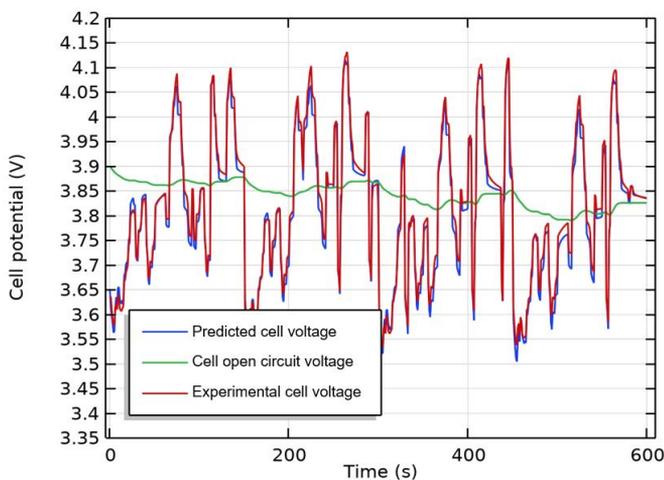


Figure 5. Cell voltage prediction

Figure 5 illustrates the predicted cell voltage (blue line), experimental cell voltage (red line), and cell open circuit voltage (green line) over a 600-second simulation period. The predicted cell voltage closely tracks the experimental cell voltage, with minor deviations during peaks and troughs, demonstrating the model's accuracy in capturing battery performance under dynamic load conditions. The green OCV line remains relatively stable, representing the cell's equilibrium voltage in the absence of current. The alignment between the predicted and experimental voltages across various load changes indicates that the lumped parameter model provides reliable predictions, with minimal error. This strong correlation validates the model's effectiveness in real-time battery management applications, where accurate voltage predictions are essential for monitoring, quality control, and optimization of battery performance.

3.4 Discussions

The results of this study underscore the effectiveness of the lumped parameter model in predicting lithium-ion battery performance under dynamic loading conditions, validating its potential for practical applications in battery production and management. By simplifying the model to focus on key overpotentials ohmic, activation, and concentration the approach offers a streamlined yet accurate prediction of cell voltage with minimal computational demand. This simplified model addresses the complexity and cost challenges associated with traditional battery models that require extensive knowledge of internal chemistry and thermal dynamics. The comparison between the predicted and experimental cell voltages, as shown in Figures 3 and 5, demonstrates the model's ability to closely replicate real-world battery behavior across various load conditions. The minor discrepancies observed in peak and trough values are expected, as the lumped parameter model simplifies certain internal dynamics to maintain computational efficiency. Despite these small deviations, the overall alignment suggests that the model is robust enough for real-time performance prediction, a critical requirement in high-throughput production environments where rapid quality control and operational adjustments are essential. The voltage loss analysis, depicted in Figures 2 and 4, further highlights the model's value by breaking down the contributions of each type of overpotential. Ohmic losses are immediate and relatively stable, driven by internal resistance, while activation and concentration losses fluctuate based on current and state of charge (SOC). This breakdown provides valuable insights for production management, as understanding these losses allows for targeted interventions to optimize efficiency and extend battery life. For instance, minimizing activation overpotentials through improved electrode materials could reduce voltage drops during high-current applications, thereby enhancing overall battery efficiency. From a production management perspective, the model's low computational requirements and accuracy enable faster cycle times by reducing the need for extensive calibration. This efficiency facilitates the integration of the model into real-time performance monitoring systems, where continuous assessment of voltage can detect potential issues early in the production process. Moreover, the ability to accurately simulate SOC and predict overpotentials makes the model highly applicable for quality assurance, as manufacturers can identify batteries that may exhibit performance inconsistencies over time. The study's findings also suggest broader implications for the application of

simplified models in energy storage technologies. By focusing on essential parameters and overpotentials, the lumped parameter model demonstrates that reliable battery performance prediction does not always require complex, detailed models. This approach aligns well with the demands of EVs and renewable energy storage systems, where operational efficiency, scalability, and cost-effectiveness are key. Furthermore, the insights gained from this model could inform future battery design, potentially guiding materials research and engineering efforts aimed at reducing specific types of voltage losses. In summary, the lumped parameter model offers a practical, scalable, and accurate tool for lithium-ion battery performance prediction, with demonstrated value for production management. Its streamlined design allows for real-time applications, addressing both quality control needs and operational efficiency in manufacturing environments. Future research could further enhance the model by refining parameters to capture peak and trough discrepancies, potentially improving its accuracy for even more demanding applications.

The lumped parameter model offers a practical tool for lithium-ion battery performance prediction, but several limitations may impact its real-world applicability, especially in demanding applications like EVs and large-scale energy storage. The model simplifies internal battery dynamics by focusing on three primary overpotentials ohmic, activation, and concentration while omitting complex thermal and electrochemical interactions, leading to potential inaccuracies under extreme or variable conditions. It also shows limited accuracy during peak power demands and lacks considerations for battery aging, which can affect prediction reliability over time. While basic temperature dependencies are included, the model does not fully address the impact of fluctuating or extreme temperatures, which significantly influence battery behavior. Additionally, the model's sensitivity to parameter calibration may limit its flexibility across different battery types and operating scenarios, as each new application might require recalibration. Importantly, the model does not account for safety-critical events, such as thermal runaway or internal short circuits, making it insufficient as a standalone solution in high-risk applications. Despite these limitations, the model remains valuable for controlled environments, such as production and quality control, though enhancements in thermal modeling, aging considerations, and transient response would improve its broader applicability.

4. CONCLUSIONS

This study demonstrates the effectiveness of a lumped parameter model in predicting lithium-ion battery performance, highlighting its potential for use in production management and quality control. By focusing on key overpotentials ohmic, activation, and concentration the model provides accurate voltage predictions with minimal computational demand, making it suitable for real-time applications. The close alignment between the predicted and experimental cell voltages validates the model's accuracy, with only minor discrepancies observed at peak and trough values. Voltage loss analysis further underscores the model's ability to capture essential battery dynamics, offering insights into how different types of overpotentials affect overall performance. However, the study also reveals certain limitations. The model's simplified approach does not fully capture complex internal battery interactions, transient

responses under extreme conditions, or long-term aging effects. While the model includes basic temperature dependencies, it lacks detailed thermal modeling and does not account for safety-critical events, which limits its applicability in high-stakes applications such as EVs and large-scale energy storage systems. Overall, the lumped parameter model offers a practical, computationally efficient solution for applications where fast, reliable performance prediction is essential, particularly in controlled environments. Future work could focus on enhancing the model's accuracy by incorporating aging effects, refining transient response under peak conditions, and adding detailed thermal modeling to expand its applicability across more demanding and varied operational scenarios.

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NOMENCLATURE

E_{cell}	Cell voltage (Volts)
E_{OCP}	Open circuit potential, dependent on SOC V (Volts)
η_{IR}	Ohmic overpotential (internal resistance loss) V (Volts)
η_{act}	Activation overpotential (charge transfer loss) V (Volts)
η_{conc}	Concentration overpotential (diffusion limitation) V (Volts)
I_{cell}	Applied cell current A (amperes)
$I_{1,C}$	1C rate current, based on nominal capacity A (amperes)
$Q_{cell,0}$	Battery capacity Ah (amp-hours)
R	Universal gas constant J/(mol·K)
T	Temperature K (kelvin)
F	Faraday's constant (C/mol)
J_0	Charge exchange current density (A/m ²)
SOC	State of Charge (%)
$\tau_{difficion}$	Diffusion time constant s (seconds)
α	Empirical scaling factor for diffusion limitations
$f(T)$	Temperature-dependent function for ohmic loss
$g(SOC)$	SOC-dependent function for activation overpotential
$h(T)$	Temperature-dependent function for activation loss