HYDROGEN, FUEL CELL & ENERGY STORAGE

Electrochemical simulation of lithium-ion batteries: a novel computational approach for optimizing performance

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Abstract

The accurate simulation of lithium-ion batteries is crucial for optimizing their performance, increasing their lifespan, and mitigating environmental concerns, as they play a vital role in powering electric vehicles, renewable energy systems, and portable electronics. This research presents a novel computational technique for simulating the internal processes of lithium-ion batteries, focusing on the electrochemical equilibrium and dynamics of these batteries. By leveraging the electrochemical method and simplifying complex differential equations through logical assumptions, the study develops a versatile tool for predicting the temporal and spatial distribution of electrode concentration, potential, and electrolyte dynamics in one dimension. The computational approach, executed in a C++ programming environment using computational fluid dynamics and the finite volume method, enables the simulation of diverse lithium-ion batteries. The research addresses the challenges posed by these batteries, including the quest for increased energy and power density, effective heat management, and control and monitoring complexities. By providing valuable insights into optimizing battery performance, this study contributes to the development of sustainable energy storage solutions. The proposed approach has the potential to shape a sustainable energy narrative, particularly in the context of all-electric and hybrid vehicles, and mitigating environmental concerns.

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1 Introduction

The integration of renewable energy sources, such as solar and wind power, into the power grid is hindered by their variability, making energy storage solutions crucial for ensuring consistent power delivery. Lithium-ion batteries (LIBs) have emerged as a leading technology due to their exceptional energy density, prolonged lifespan, and remarkable versatility [1]. They are ideal for powering portable electronic devices, and their success has spurred rapid advancements, making them increasingly viable for electric vehicles and grid-scale energy storage applications [2]. As the demand for renewable energy continues to grow, advancements in LIB technology will play a critical role in enabling a more sustainable and efficient energy infrastructure. However, further research and development are necessary to overcome remaining challenges and unlock their full potential in supporting the widespread adoption of renewable energy sources [3]. However, despite their numerous advantages, LIBs are not without challenges. One of the primary concerns is ensuring safety. The presence of flammable electrolytes within LIBs raises potential safety hazards in cases of overheating or damage. Mitigating these risks and developing inherently safer battery chemistries remains an active area of research. Another challenge associated with LIBs is their limited energy density compared to theoretical limits [4]. While current LIBs offer significant improvements over older technologies, there is still room for enhancement. Continued research focuses on developing novel electrode materials and electrolytes to achieve even higher energy densities, enabling longer driving ranges for electric vehicles and increased storage capacity for grid applications. Finally, the issue of cost remains a hurdle for widespread LIB adoption, particularly in large-scale energy storage applications. The raw materials used in LIBs, such as lithium and cobalt, can be expensive. Developing cost-effective extraction and processing methods, as well as exploring alternative materials, are crucial for making LIBs more economically viable [5].

Optimizing LIB performance and lifespan requires understanding internal electrochemical processes. These processes involve complex interactions between electrodes, electrolyte, and separator. Direct observation of internal dynamics is challenging due to the battery's opaque nature and transient reactions [6]. Computational modeling and simulation provide valuable insights into internal behavior. Simulations can predict voltage response, capacity fade, and thermal behavior under various operating conditions. This capability enables researchers to virtually test design parameters and optimize battery performance. Simulations can also model degradation mechanisms, such as lithium plating and electrolyte decomposition. This understanding guides the development of strategies to mitigate degradation and extend battery lifespan [7]. Computational simulations can also screen and optimize new electrode materials and electrolytes. This accelerates the discovery and development of next-generation LIBs [8].

This research introduces a novel computational technique to overcome the challenges in LIB development by simplifying complex differential equations and facilitating efficient numerical solutions.

- Simplified Governing Equations: The technique simplifies complex differential equations that govern the behavior of LIBs through logical assumptions, making it possible to obtain computationally efficient numerical solutions. The governing equations for LIBs are complex due to nonlinear relationships, coupled phenomena, and multiple scales, but the technique reduces this complexity by neglecting non-essential terms, linearizing nonlinear relationships, and assuming steady-state conditions.
- Versatile Simulation Tool: A C++-based simulation developed using CFD and the FVM, enabling the simulation of diverse LIB configurations. This tool allows users to model and simulate various LIB designs, including different electrode materials, electrolyte compositions, and cell geometries, under various operating conditions.
- Insights into Optimizing Battery Performance: The technique provides valuable insights into optimizing battery performance by simulating the complex interactions between electrode concentration, potential, and electrolyte dynamics, allowing researchers and engineers to identify key factors that impact battery performance.
- Addressing LIB Challenges: The research addresses several key challenges in LIB development, including the need for higher energy and power density, effective heat management, reduced costs, and simplified control and monitoring systems. LIBs are limited by their energy density, which affects their ability to power devices for extended periods, and their power density, which impacts their ability to deliver high currents.
- Linearization Method: A linearization method is developed to solve nonlinear equations that arise in the modeling of LIBs, which is a crucial step in ensuring the accuracy and efficiency of the simulation process. Nonlinear equations can be

challenging to solve, as they often require iterative methods that can be computationally expensive and prone to instability. The linearization method enables the use of the Thomas algorithm, a highly efficient method for solving tridiagonal systems of equations, which is a common form of linear equations that arise in LIB modeling.

This novel computational technique has the potential to revolutionize the development of high-performance LIBs by providing a powerful tool for simulating battery processes with unprecedented speed and accuracy.

The paper is structured as follows. Section 2 provides a comprehensive literature survey on modeling Lithium-Ion Battery (LIB) behavior, summarizing the current state of knowledge and identifying gaps in existing research. Section 3 introduces the proposed method, providing a detailed description of the methodology, including mathematical formulations, assumptions, and numerical techniques used. The proposed method is then validated through numerical simulations in section 4, demonstrating its superiority over current methods and highlighting its accuracy and efficiency. Finally, the concluding section (section 5) summarizes the key findings, emphasizes the importance of the proposed method in the field of LIBs, and highlights its potential applications and implications, including its potential to accelerate the development of high-performance LIBs.

2 Modeling lithium-ion battery behavior

Understanding the behavior of LIBs is crucial for optimizing their performance, ensuring safe operation, and maximizing their lifespan. To achieve this, researchers and developers rely on various modeling approaches, each with its strengths and limitations. This section provides an overview of three prominent modeling techniques used to analyze lithium-ion battery behavior: electrochemical models, equivalent circuit models, and data-driven models. By examining the strengths and limitations of each approach, we can better understand their applications and potential in advancing lithium-ion battery research and development.

2.1 Electrochemical models

Electrochemical models have emerged as a powerful tool for understanding and optimizing the intricate processes that occur within LIBs. By accounting for the interplay between chemical reactions and physical phenomena, these physics-based models enable researchers to simulate various factors, including lithium-ion concentration, potential distribution, and heat generation [9]. As a result, they provide a comprehensive understanding of the internal workings of a battery, capturing the fundamental relationships between electrode materials, electrolyte properties, and battery performance. Electrochemical models offer a powerful tool for understanding battery behavior, providing detailed insights and predictive capabilities that enable researchers to optimize battery design and operation for specific applications. By simulating battery behavior under various conditions, these models facilitate virtual prototyping, accelerating development and reducing the need for physical experimentation [10].

However, they also have limitations, including high computational costs for complex simulations, reliance on accurate input parameters, and the challenge of validating models against experimental data due to the difficulty of measuring internal battery variables. [11] reviews the current state of electrochemical modeling and parameterization techniques for LIBs, highlighting the importance of accurate modeling and parameterization for optimal battery performance, longevity, and safety. [12] proposes a state-of-health estimation method for LIBs in electrified vehicles using a reduced-order electrochemical model that balances accuracy and computational efficiency. [13] provides a critical review of efficient parameter estimation methodologies for electrochemical models of Lithium-Ion cells, evaluating their strengths, limitations, and applicability in various scenarios.

2.2 Equivalent circuit models (ECMs)

Equivalent circuit models (ECMs) provide a pragmatic approach to analyzing lithium-ion battery behavior, prioritizing simplicity and computational efficiency over detailed physics-based representations. By representing the battery's electrical characteristics as a network of basic electrical components, such as resistors, capacitors, and voltage sources, ECMs offer a simplified yet effective way to understand battery behavior [14]. ECMs excel in real-time applications, offering speed and efficiency in predicting voltage and current behavior under various operating conditions, making them valuable for battery management systems. However, their simplicity comes at the cost of lacking insight into internal battery processes, such as lithium-ion concentration and heat generation, and limited predictive power for complex phenomena like battery degradation and extreme operating conditions [15]. While ECMs are practical for understanding electrical behavior, they are limited in providing comprehensive insights, which are better addressed by electrochemi-

cal models that offer a more detailed understanding of underlying physical and chemical processes. [16] paper presents a physicochemical equivalent circuit model for LIBs, which combines the simplicity of equivalent circuit models with the physical insights of electrochemical models, and evaluates its performance through experimental validation. [17] compares the performance of various electrical equivalent circuit models in capturing the hysteresis effect of Lithium Iron Phosphate batteries, evaluating their accuracy and computational efficiency in simulating battery behavior. [18] proposes a dynamic equivalent circuit model to estimate the state-of-health of LIBs, which can accurately capture the battery's dynamic behavior and degradation mechanisms.

2.3 Data-driven models

Data-driven models offer a novel approach to understanding lithium-ion battery behavior, leveraging machine learning algorithms to uncover hidden patterns within vast amounts of experimental data. This approach proves highly effective in capturing complex relationships between various operating conditions and the resulting performance metrics of a battery [19]. By bypassing the need for a deep understanding of the underlying electrochemical processes, data-driven models can identify crucial relationships between operating conditions and battery performance, even in situations where the intricate details of these processes are not fully elucidated [20]. Data-driven models offer a valuable approach to understanding lithium-ion battery behavior, capturing intricate, non-linear relationships and subtle interactions between factors and performance metrics. By training on historical data, they can estimate battery health and predict remaining useful life with greater accuracy, optimizing performance, ensuring safe operation, and maximizing lifespan. However, their effectiveness relies on high-quality and sufficient data, and biased or incomplete data can lead to inaccurate predictions.

Additionally, these models often lack interpretability, making it difficult to understand the underlying battery processes [21] presents a data-driven approach for estimating the state-of-health of LIBs, which utilizes internal resistance as a key indicator of battery degradation and health. [22] proposes a data-driven predictive prognostic model using a deep learning algorithm to accurately predict the remaining useful life of LIBs based on their charging and discharging cycles. [23] presents a data-driven modeling approach using dynamic mode decomposition to identify and predict the dynamic behavior of LIB, enabling accurate State Of Charge (SOC) and health estimation.

2.4 Comparison of modeling techniques

Table 1 summarizes the strengths and limitations of three prominent modeling techniques used to analyze lithium-ion battery behavior: electrochemical models, equivalent circuit models, and data-driven models.

Table 1. Comparison of strengths and limitations of electrochemical models, equivalent circuit models, and data-driven models for battery modeling

Modeling Technique	Strengths	Limitations
Electrochemical Models	Comprehensive understanding of internal battery processes, detailed simulations, and predictive capability	Computationally expensive, requires accurate input parameters, and challenging to validate
Equivalent Circuit Models	Simplified and efficient, ideal for real-time applications, and accurate predictions of voltage and current behavior	Lacks detailed understanding of internal battery processes, limited predictive power for complex phenomena
Data-Driven Models	Captures complex relationships, excels at learning from data, and valuable for battery management systems	Effectiveness depends on data quality and quantity, lacks interpretability, and limited understanding of fundamental battery processes

Electrochemical models (also known as physics-based models) are fundamentally more comprehensive and scientifically rigorous. These models are built on first-principles equations derived from electrochemical kinetics, thermodynamics, and transport phenomena. They provide a deep, mechanistic understanding of the internal state and processes of batteries, such as ion concentration gradients, electrode kinetics, and temperature effects. This level of detail is crucial for the accurate simulation of battery behavior, allowing researchers to investigate performance, degradation, and failure mechanisms with high precision. However, their complexity requires extensive experimental data for parameterization and high computational resources, making them less practical for real-time applications or when computational efficiency is needed. In contrast, equivalent circuit models (ECMs) and data-driven models operate at a different level. ECMs simplify battery behavior into a network of resistors, ca-

pacitors, and voltage sources, providing a balance between accuracy and computational efficiency. They are widely used for system-level simulations and real-time battery management systems (BMS) due to their simplicity and ease of implementation.

However, ECMs lack the ability to capture detailed internal electrochemical processes and are generally suitable for short-term predictions rather than long-term performance analysis. Data-driven models, leveraging machine learning and statistical techniques, further abstract the battery system. These models rely on historical and real-time data to predict battery behavior, making them powerful tools for applications where vast amounts of data are available and real-time performance is critical. However, they are inherently limited by the quality and scope of the training data and do not provide the physical insight necessary for understanding the root causes of battery degradation or failure. Given these differences, it is important to emphasize that electrochemical models remain the gold standard for in-depth battery analysis and research, providing the foundation for understanding fundamental mechanisms. The use of ECMs and data-driven models is often motivated by specific practical needs, such as the requirement for real-time monitoring or the constraints of computational resources. Therefore, these techniques should be seen as complementary approaches, rather than equivalent alternatives, to electrochemical modeling. This clarification ensures that the table reflects the hierarchical nature of these methods and the context in which each is appropriately applied. Therefore, electrochemical models are the preferred choice for advancing lithium-ion battery research and development.

3 Methodology

The behavior of electrochemical systems is governed by a complex interplay of physical and chemical processes. To develop a deeper understanding of these systems, it is essential to formulate a mathematical framework that captures the underlying mechanisms. In this section, we present a set of coupled partial differential equations that describe the retention of electric charge and species in the electrode and electrolyte. These equations provide a fundamental basis for understanding the behavior of electrochemical systems, including the transport of ions and electrons, the distribution of electrical potential, and the dynamics of species concentrations. By solving these equations, we can gain valuable insights into the performance and limitations of electrochemical devices, and inform the design of optimized systems for a wide range of applications. The retention of electric charge in the electrode is governed by:

$$\sigma^{\text{eff}} \frac{d^2\phi_s}{dx^2} - j^{Li} = 0 \tag{1}$$

Equation (1) represents Ohm's Law within the electrode. σ^{eff} (effective conductivity) relates the current density (j^{Li}) to the electrical potential gradient ($\frac{d^2\phi_s}{dx^2}$) within the electrode. The retention of electric charge in the electrolyte is described by:

$$K^{\text{eff}} \frac{d^2\phi_e}{dx^2} + K_D^{\text{eff}} \frac{d^2}{dx^2} \log_e(c_e) + j^{Li} = 0 \tag{2}$$

Equation (2) reflects charge neutrality within the electrolyte. K^{eff} (effective conductivity) relates the j^{Li} to $(\frac{d^2\phi_s}{dx^2})K_D^{\text{eff}}$ (effective diffusion coefficient) and c_e (electrolyte concentration) account for the influence of concentration gradients on the potential distribution through the term $\frac{d^2}{dx^2}(\log_e(c_e))$.

The retention of species in the electrode is presented as:

$$\frac{\partial(\varepsilon_s c_s)}{\partial t} = \frac{j^{Li}}{F} \tag{3}$$

Equation (4) describes the change in the electrode species concentration (c_s) over time (t) due to j^{Li}. ε_s (volume fraction of the solid phase in the electrode) and F (Faraday's constant) account for the conversion between current and concentration changes. The retention of species in the electrolyte is described by:

$$\varepsilon_e \frac{\partial c_e}{\partial t} = D^{\text{eff}} \frac{\partial^2 c_e}{\partial x^2} + \frac{1 - t_+^\circ}{F} j^{Li} \tag{4}$$

Equation (4) describes the change in c_e over t due to diffusion (D^{eff}) and j^{Li}. ε_e (volume fraction of the electrolyte) and t_+° (transference number) account for the transport of Lithium ions within the electrolyte.

This research focuses on four key variables that are critical to understanding the behavior of electrochemical systems: electrolyte concentration, electrode concentration, electrode potential, and electrolyte potential. Accurately predicting these variables is vital for optimizing the performance of LIBs. The model used in this study makes two key assumptions: a constant temperature, which is a reasonable assumption given the typical operating conditions of LIBs, and no electrolyte movement within the battery, which is a valid assumption due to the battery's tight packaging and the pressure on the electrodes and electrolyte solution. This latter assumption simplifies the continuity equations by eliminating the need for an advection term [24].

The equations that govern electrochemical systems are intricate and nonlinear, with only the concentration-related equations exhibiting time-dependent behavior. While the other equations are

solved separately at each time step, the strong interconnection between them means that all variables will have both spatial and temporal dependencies. To tackle these complex equations, numerical methods are essential, specifically Computational Fluid Dynamics (CFD) and the finite volume method. The CFD approach requires iterative solutions, but the nonlinearity of the equations can lead to instability and challenges in the solution process [25]. To address the challenges posed by the nonlinear equations, a linearization step is necessary to ensure a stable solution process. This linearization transforms the discretized system of equations into a tridiagonal system, which can be efficiently solved using the Thomas algorithm. This approach provides a powerful tool for understanding the behavior of electrochemical systems, offering valuable insights into the underlying mechanisms that govern lithium-ion battery behavior. By solving these equations, researchers can gain a deeper understanding of the complex processes at play, ultimately informing the design of optimized battery systems for a wide range of applications.

4 Simulations

This section presents the results of the CFD simulation, which aimed to investigate the behavior of a lithium-ion battery. The simulation outputs include the electrolyte concentration, electrode concentration, electrode potential, and electrolyte potential along the cell length, as well as the cell voltage during discharge. These results provide valuable insights into the battery's performance and efficiency, and were validated by comparing them with reference results [26].

4.1 Cell voltage

The Cell Voltage plot is crucial in this research as it validates the simulation approach by comparing with reference results, provides insights into battery performance for optimization of design and operation, is essential for developing sustainable energy storage solutions, plays a vital role in the electrification of transportation by optimizing battery performance for electric vehicles, and serves as a benchmark for comparing different battery designs, materials, and operating conditions, ultimately contributing to the development of sustainable energy storage solutions.

The cell voltage plot in Figure 1 compares the simulated results with the numerical solution results from a referenced article [26], showing the cell voltage during discharge, which is a critical parameter in understanding the battery's performance, with a discharge time of 1 hour and a current of 1.75 $\mathrm{mA/cm^2}$. As the capacity increases, the cell voltage decreases, with the maximum capacity for the cell being 3.92, indicating that the battery's capacity is directly related to the amount of lithium ions that can be stored and released during discharge. The relationship between capacity and cell voltage has significant implications for battery performance, with a higher cell voltage indicating a higher SOC and a lower cell voltage indicating a lower SOC, and the rate of decrease in cell voltage during discharge affecting the battery's ability to supply power and energy.

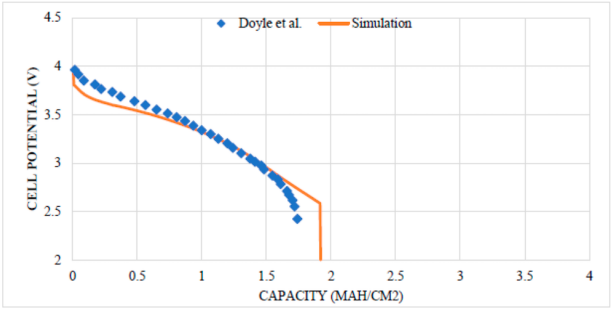

Fig. 1. Comparison of voltage calculation results using numerical modeling and reference results [26]

The sharp cut-off value observed in Figure 1 represents the predefined capacity limit where the battery is considered to reach the end of discharge. This simulation uses a specific voltage threshold to determine when the cell is depleted. Such sharp cut-offs are often implemented in models to mimic protective circuitry found in real battery systems, which prevents over-discharge and potential damage. The simulation parameter is set based on standard lithium-ion battery specifications to align with realistic operational safety practices. The comparison with the numerical solution results serves as a validation of the simulation results, ensuring that the simulation model is accurate and reliable, and building confidence in the simulation results to make informed decisions about battery design and performance.

4.2 Electrolyte concentration

The electrolyte concentration plot is vital in this research as it provides insights into lithium-ion transport, identifies capacity limitations, informs electrode design optimization, reveals aging mechanisms, helps mitigate safety risks, enhances battery efficiency, and guides material selection,

Figure 2 illustrates the lithium-ion distribution within the battery during discharge, showing the concentration of lithium-ions and other materials along the dimensionless cell length. The plot reveals that

lithium-ions separate from the negative electrode, indicating the presence of Li^+ ions, and exhibit slightly greater concentration changes in the negative electrode during discharge. This highlights the critical role of the negative electrode in battery performance, as its concentration changes directly impact the battery's capacity, power output, and efficiency. By analyzing the lithium-ion distribution and concentration changes, researchers can optimize the negative electrode design, leading to improved battery performance and efficiency, and gain a deeper understanding of the underlying mechanisms driving battery performance, ultimately enabling the development of more advanced and efficient battery technologies.

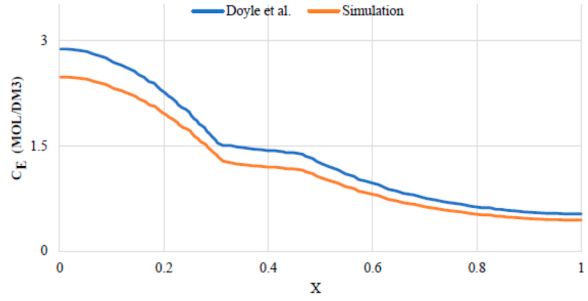

Fig. 2. Comparison of electrolyte concentration calculation results using numerical modeling and reference results [26]

4.3 Electrolyte potential

The electrolyte potential plot is crucial in this research as it provides insights into electrolyte behavior, identifies potential losses, informs electrolyte design optimization, reveals underlying electrochemical reactions, and helps improve battery safety by mitigating thermal runaway risks, ultimately contributing to the development of more efficient, safe, and high-performance batteries.

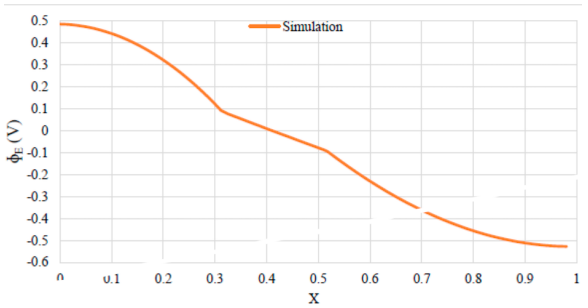

Fig. 3. Electrolyte potential calculation results using numerical modeling

The electrolyte potential plot in Figure 3 provides a critical insight into the internal workings of the lithium-ion battery, showing the electrolyte potential along the dimensionless cell length, which is a key parameter in understanding the electrochemical reactions that occur within the battery. The continuous production of lithium-ions in the cathode and their consumption on the anode side result in a potential gradient in the electrolyte, driving the movement of lithium-ions from the cathode to the anode, which is essential for the battery's ability to supply power. Throughout the electrochemical reactions, the electrolyte potential on the anode side will consistently be higher than that on the cathode side, due to the electrochemical reaction, and a uniform gradient is essential for efficient electrochemical reactions, while non-uniform gradients can lead to reduced battery performance, increased energy losses, and even safety issues. By understanding the electrolyte potential gradient, researchers can optimize battery design, improve charging and discharging rates, and enhance overall battery efficiency, gaining a deeper understanding of the underlying mechanisms that drive battery performance, which is essential for developing more advanced and efficient battery technologies.

4.4 Electrode Concentration and Electrode Potential

The electrode concentration and electrode potential plots are crucial for understanding lithium-ion transport, identifying capacity limitations, optimizing electrode design, understanding aging mechanisms, improving battery safety, and enhancing battery efficiency, as well as understanding electrode behavior, identifying potential limitations, understanding electrochemical reactions, and improving battery efficiency, ultimately contributing to the development of high-performance, safe, and efficient LIBs. Figures 4 and 5 show the temporal evolution of electrode potential and concentration, respectively. The apparent simplicity and repeated static value suggest that the chosen time frame might not capture significant changes in these parameters. The electrode potential is highly dependent on the rate of lithium-ion transport and interfacial reactions. Extending the time frame or increasing the resolution of the data points could provide more dynamic insights into the potential distribution changes within the battery. Future simulations should adjust the time frame and sampling rate to ensure that the transient behavior of the electrode potential is adequately represented.

The simulation results in Figure 4 demonstrate the electrode potential distribution along the cell length at various time points, offering valuable insights into the potential distribution within the battery. The external current is generated by the potential difference between

the anode and cathode, with the negative electrode potential set as a reference point (zero) and the positive electrode potential measured relative to it. This simplifies the analysis and provides a basis for understanding the electrochemical reactions during charging and discharging. A uniform electrode potential distribution is crucial for efficient electrochemical reactions, while non-uniform distributions can lead to reduced battery performance, increased energy losses, and safety concerns. Therefore, analyzing and optimizing the electrode potential distribution is essential for developing more efficient and safe LIBs.

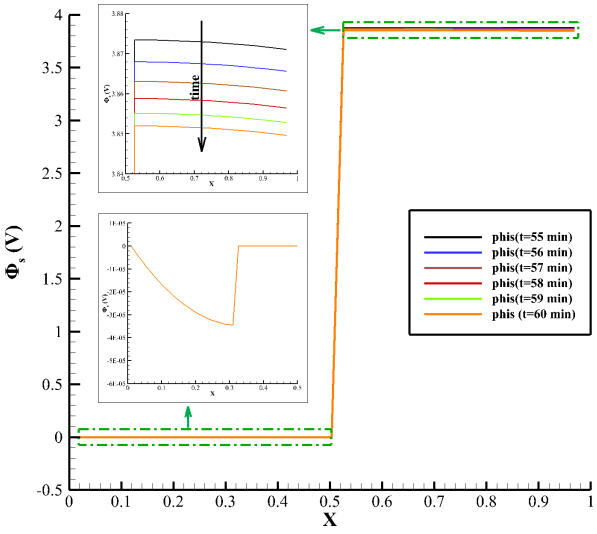

Fig. 4. Electrode potential changes at different times

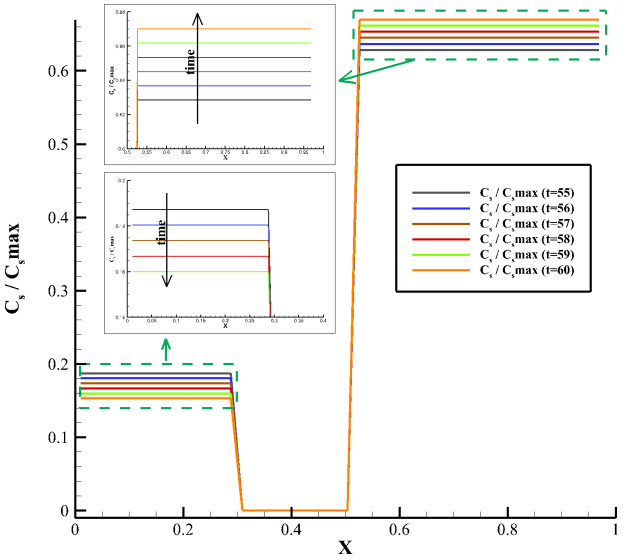

Fig. 5. Electrode concentration changes at different times

The simulation results for electrode concentration, presented in Figure 5, offer a detailed view of the electrode concentration throughout the dimensionless length of the cell during the final 5 minutes of the discharge process, revealing a noticeable increase in the SOC as time progresses, which is a critical parameter in battery performance. The plot provides valuable insights into the dynamic behavior of the battery during the discharge phase, shedding light on how the internal processes and variables change over time, and is essential for understanding the underlying mechanisms that govern battery performance. The electrode concentration dynamics reveal the complex transport of lithium ions within the battery, which affects the electrochemical reactions that occur during charging and discharging, and has significant implications for battery performance, including opportunities to optimize battery design, improve charging and discharging rates, and enhance overall battery efficiency. By analyzing the electrode concentration dynamics, researchers can gain a deeper understanding of the internal processes that drive battery behavior, ultimately leading to the development of more efficient, reliable, and sustainable LIBs.

5 Conclusion

This study introduces a pioneering computational approach that simplifies the complexities of lithium-ion battery development by breaking down intricate mathematical equations and enabling rapid numerical solutions. The research demonstrates the effectiveness of a one-dimensional simulation and modeling approach, utilizing CFD and C++ programming, in understanding the intricate behavior of LIBs. The simultaneous calculation of unknowns, including electrolyte concentration and potentials in electrodes and electrolytes, provides a comprehensive understanding of battery behavior, illuminating the complex transport of lithium ions, electrochemical reactions, and potential distributions that govern battery performance. The simulation results, presented in five figures, offer a detailed insight into the battery's internal workings, including the cell voltage, dimensionless cell length, electrolyte potential, electrode potential, and electrode concentration. These results provide valuable information for optimizing battery design, improving charging and discharging rates, and enhancing overall battery efficiency. The advantages of this simulation methodology are twofold.

Firstly, it offers a cost-effective alternative to experimental tests, which can be time-consuming and expensive. Secondly, it enables the simulation of various scenarios and conditions, allowing researchers to test and optimize different battery designs and operating conditions without the need for physical prototypes.

The findings of this study highlight the importance of continued efforts in developing accurate models to improve the performance, reliability, and sustainability of LIBs. By advancing our understanding of the underlying mechanisms that drive battery behavior, we can develop more efficient, reliable, and sustainable energy storage solutions, which are critical for the widespread adoption of electric vehicles and renewable energy systems.

Future research directions include extending the current 1D model to 2D/3D, incorporating thermal and mechanical effects, and developing machine learning algorithms for optimization. Experimental validation using advanced characterization techniques is also recommended to further improve lithium-ion battery performance, reliability, and sustainability.

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