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NUMERICAL SIMULATION AND MODELING OF ELECTROCHEMICAL PROCESSES IN LITHIUM-ION BATTERIES

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ABSTRACT

This research embarks on an illuminating exploration of electrochemical equilibrium, focusing on lithium-ion batteries, particularly lithium-ion batteries renowned for their extended lifespan. Leveraging the electrochemical method, a simulation approach rooted in physical equations, the study unveils a novel computational technique for predicting the internal processes of batteries with temporal and spatial distribution in one dimension. The method's efficiency lies in simplifying complex differential equations through logical assumptions and facilitating numerical solutions. Executed in a C++ programming environment using computational fluid dynamics and the finite volume method, the research's code becomes a versatile tool for simulating diverse lithium-ion batteries. As the calculations traverse positive electrode, negative electrode, and separator regions, the intricate dance of electrode concentration, potential, and electrolyte dynamics comes to life, promising valuable insights into optimizing battery performance. This journey into the heart of electrochemical phenomena paves the way for sustainable energy storage solutions, marking a significant stride in the realm of battery technology [1].

Keywords: Lithium-ion batteries, Electrochemical modeling, Numerical simulation, Computational fluid dynamics.

INTRODUCTION

In the realm of energy storage, batteries emerge as pivotal devices, harnessing the alchemy of chemical energy conversion into electrical power. Among these devices, lithium-ion batteries stand out due to their commendable attributes such as high energy density, lightweight composition, rapid charge/discharge capabilities, and prolonged operational life. These batteries find extensive applications in various engineering domains, notably all-electric and hybrid vehicles, contributing to mitigating environmental concerns. However, these seemingly miraculous devices face significant challenges, including the quest for increased energy and power density, effective heat management, financial considerations, and the complexities of control and monitoring. This research embarks on a scientific exploration, delving into the intricacies of lithium-ion batteries through electrochemical simulation and modeling. The objective is not merely comprehension but the creation of simulations that accurately mirror the transient behavior of batteries. Through computational efficiency and logical assumptions, the research simplifies the differential equations governing battery components, facilitating numerical solutions. Employing a C++ programming environment, computational fluid dynamics, and the finite volume method, the interconnected governing equations are solved, offering a versatile tool for simulating diverse lithium-ion batteries. This study endeavors to address the challenges posed by these batteries, positioning simulations as a cornerstone in shaping a sustainable energy narrative [2].

MATERIALS AND METHODS

In this research, we have utilized a model that considers only the spatial changes of the desired quantities along the length of the cell (in the x-direction) and neglects variations in other directions. The final form of the one-dimensional equations for lithium-ion batteries in this study is written as follows [1]. In this study, the primary unknowns include electrolyte concentration, electrode concentration, electrode potential, and electrolyte potential. The model under investigation in this research assumes a constant temperature. Since there is no electrolyte movement in the lithium-ion battery due to the tight packaging of the battery and the pressure on the electrodes and electrolyte solution, the fluid velocity in such batteries is considered zero.

Table 4: List of Equations in Li-ion Batteries

SN	Name	Equation
1	Retention of electric charge in the electrode	$\sigma^{eff}\frac{d^2\phi_s}{dx^2} - j^{Li} = 0$
2	Retention of electric charge in the electrolyte	$\kappa^{\mathrm{eff}}\frac{\mathrm{d}^2\phi_\mathrm{e}}{dx^2} + \kappa_\mathrm{D}^{\mathrm{eff}}\frac{\mathrm{d}^2}{\mathrm{dx}^2}(\log_\mathrm{e}(\mathrm{c_e})) + \mathrm{j}^{\mathrm{Li}} = 0$
3	Retention of species in the electrode	$\frac{\partial(\varepsilon_\mathrm{s}\,\mathrm{c_s})}{\partial \mathrm{t}} = \frac{\mathrm{j}^{\mathrm{Li}}}{\mathrm{F}}$
4	Retention of species in the electrolyte	$\varepsilon_e\frac{\partial c_e}{\partial t} = D^{eff}\frac{\partial^2 c_e}{\partial x^2} + \frac{1-t_+^\circ}{F}j^{Li}$

Therefore, there will be no advection term in the continuity equations. On the other hand, among the mentioned equations, only those related to electrolyte and electrode concentrations have time-dependent terms, and the other equations are solved independently of time in each time interval. However, due to the strong coupling between these equations, all unknowns will have both spatial and temporal dependencies [3]. To solve the equations written in Table 1, numerical solution methods are necessary, particularly using Computational Fluid Dynamics (CFD) and employing the finite volume method. The Computational Fluid Dynamics method is an implicit approach, and since the governing equations are nonlinear, iterative methods are required to find the solution. However, the presence of nonlinear equations can lead to instability in repeated iterations, posing challenges in the solution process. Therefore, for solving with the Computational Fluid Dynamics method, these equations need to be linearized. After linearization of the system of equations resulting from discretization, a tridiagonal system of equations will be obtained, which can be solved with the Thomas algorithm [4].

RESULTS AND DISCUSSION

In this study, using computational fluid dynamics, the electrolyte concentration along the cell length, electrode concentration over time, electrode potential along the cell length, and electrolyte potential along the cell length have been determined. Furthermore, for validation purposes, the obtained results from this research have been compared with the reference results [5].

In Figure 1, the cell voltage during discharge is compared with the numerical solution results in the referenced article [5]. The discharge time is set to 1 hour, and the current is considered as 1.75 mA/cm². As the capacity increases, the cell voltage decreases, with the maximum capacity for the cell being 3.92.

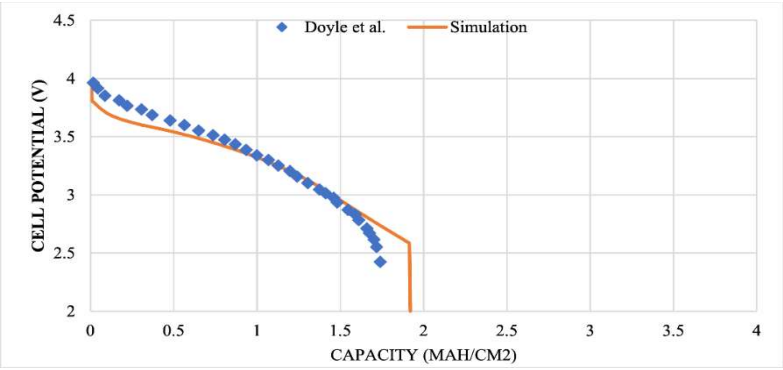

Figure 33: Comparison of voltage calculation results using numerical modeling and reference results [5].

Figure 2 illustrates the electrolyte concentration along the cell during discharge, considering a discharge time of 1 hour. As evident from the graph, there is a decrease in concentration along the cell during discharge. Additionally, dimensionless cell length is depicted in Figure 2. Lithium-ions separate from the negative electrode, implying the presence of Li^+. Conversely, in the cathode, the behavior is characterized by lithium-ions and observed materials, showing slightly greater concentration changes in the negative electrode during discharge. These variations underscore the significance of the negative electrode in the design.

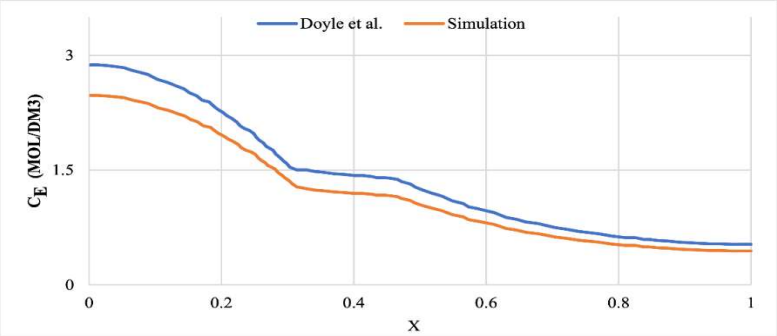

Figure 34: Comparison of electrolyte concentration calculation results using numerical modeling and reference results [5].

In Figure 3, the electrolyte potential along the dimensionless cell length is presented. The continuous production of lithium-ions in the cathode and their consumption on the anode side result in a potential gradient in the electrolyte. Under the influence of this field, lithium-ions move from the cathode towards the anode. Throughout electrochemical reactions, the electrolyte potential on the anode side will consistently be higher than that on the cathode side.

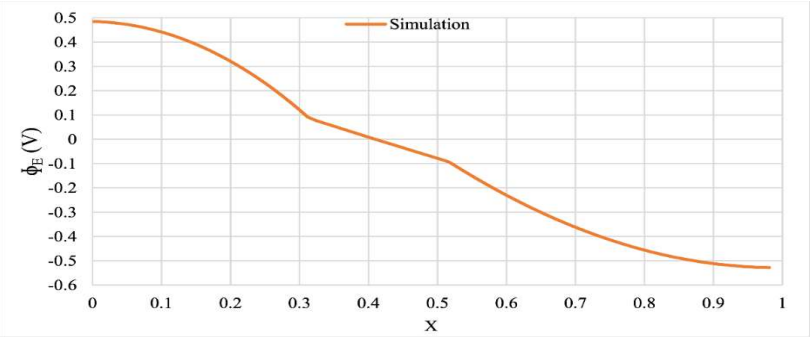

Figure 35: Electrolyte potential calculation results using numerical modeling.

Simulation results for electrode potential: The electrode potential along the dimensionless cell length is illustrated at different time points in Figure 4. The external current of a cell is generated due to the potential difference between the anode and cathode. Typically, the potential of the negative electrode is considered zero, and the potential of the positive electrode is measured relative to it. With this assumption, the positive electrode potential will always be at a higher level compared to the negative electrode on the surface.

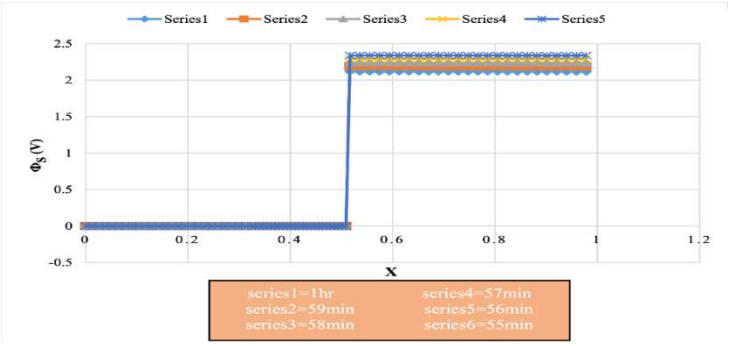

Figure 36: Electrode potential changes at different times.

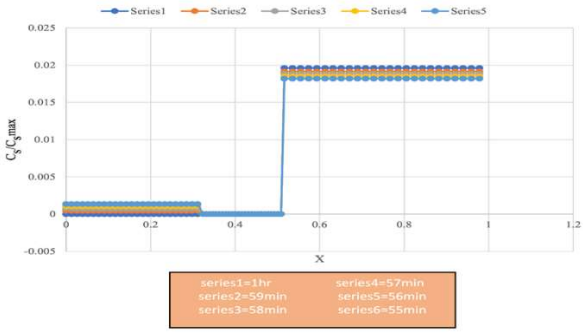

Figure 37: Electrode concentration changes at different times.

Simulation results for electrode concentration: Figure 5 provides a detailed view of the electrode concentration throughout the dimensionless length of the cell in the final 5 minutes of the discharge process. The State of Charge (SOC), a critical parameter in battery performance, exhibits a noticeable increase as time progresses. This temporal evolution of electrode concentration is a key aspect in understanding the dynamic behavior of the battery during the discharge phase, shedding light on how the internal processes and variables change over time.

CONCLUSIONS

In conclusion, the one-dimensional simulation and modeling approach employed in this research, utilizing Computational Fluid Dynamics and C++ programming, offers a cohesive solution to the complex and nonlinear equations governing lithium-ion batteries. The simultaneous calculation of unknowns, including electrolyte concentration and potentials in electrodes and electrolytes, provides a comprehensive understanding of battery behavior. This simulation methodology proves advantageous in circumventing the cost challenges associated with experimental tests. The findings underscore the importance of continued efforts in developing accurate models to bridge the performance gap between current lithium-ion batteries and their idealized counterparts.

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