

## MODELING OF ELECTROCHEMICAL DYNAMICS IN LITHIUM TITANATE OXIDE BATTERIES

<sup>1\*</sup> Elham Hasani, <sup>2</sup> Peimaneh Shirazi, <sup>3</sup> Sina Eghbal, <sup>4</sup>Farschad Torabi

<sup>1</sup> Department of Chemical and Environmental Engineering, University of Cincinnati, Cincinnati, OH 45221, United States

<sup>2</sup> Department of Mechanical and Manufacturing Engineering, Ontario Tech University, Oshawa, ON L1G 0C5, Canada

<sup>3</sup> Department of Electrical and Computer Engineering, University of Cincinnati, Cincinnati, OH 45221, United States

<sup>4</sup> Battery and Energy Generators Research Lab, K.N. Toosi University of Technology, Tehran, Iran

\* hasaniem@mail.uc.edu

### ABSTRACT

In the rapidly evolving domain of energy storage, lithium titanate (LTO) batteries have emerged as a prominent contender due to their exceptional recharge capabilities and cycle life. This research presents a deep dive into the electrochemical behaviors inherent to LTO batteries, facilitated by a custom computational framework coded in C++. Beyond just modeling, our analysis unravels the multifaceted interactions within LTO cells, elucidating factors that influence their operational robustness and efficiency. Through our refined algorithmic methodology, we ascertain critical performance metrics, degradation patterns, and thermal behaviors specific to LTO technology. This comprehensive study augments our current knowledge about LTO battery systems, paving the way for optimized designs and broader applications in next-generation energy solutions.

**Keywords:** Lithium titanate (LTO) batteries, Electrochemical behaviors, Computational framework

### INTRODUCTION

In the landscape of power storage solutions, batteries have become indispensable tools, acting as the nexus where chemical energy transitions into electrical output. Among the vast array of available choices, lithium titanate (LTO) batteries have garnered attention for their unique features, including superior charging rates, exceptional stability, and an extended lifespan. These characteristics make LTO batteries highly sought after in several technological sectors, particularly in renewable energy systems and modern transport modalities, emphasizing their role in promoting green initiatives. Nevertheless, even with their noteworthy advantages, LTO batteries face a myriad of challenges. These encompass the pursuit of enhanced storage capacity, efficient thermal regulation, cost-effectiveness, and intricate management and diagnostic mechanisms. This investigation takes a deep dive into the sophisticated world of LTO batteries, harnessing the power of electrochemical modeling to elucidate their nuanced operations. Our aim extends beyond mere understanding, focusing on the development of models that capture the dynamic essence of LTO battery systems. By streamlining the governing equations and adopting a practical approach, this research facilitates accessible numerical interpretations. Utilizing the robustness of C++ as the coding platform, coupled with intricate algorithmic strategies, the study resolves the composite equations integral to LTO functionality. With this research, we aim to tackle the inherent challenges of LTO batteries, highlighting the pivotal role of precise modeling in steering the future of sustainable energy solutions [1] [2].

### MATERIALS AND METHODS

In our study, we employed a model focusing on the spatial alterations of the targeted variables along the cell's length (in the x-direction), omitting deviations in alternate directions. The resulting one-dimensional formulations for lithium titanate batteries are presented as follows [3].

Within the scope of our research, the primary variables are electrolyte density, electrode density, electrode charge potential, and electrolyte charge potential. The model employed here works under the presumption of an invariant temperature. Given the dense assembly of the battery coupled with the force exerted on the electrodes and electrolyte solution, it's understood that there's negligible electrolyte movement within the lithium titanate battery. As such, the fluid's speed is approximated to be nil, eliminating any advection term from the continuity equations. Among the equations, solely the ones corresponding to the electrolyte and electrode densities are time-variant, while others are evaluated devoid of time within each respective time frame.

Table 7: Table of equations in LTO 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	$\kappa^{eff} \frac{d^2 \phi_e}{dx^2} + \kappa_D^{eff} \frac{d^2}{dx^2} (\log_e(c_e)) + j^{Li} = 0$
3	Retention of species in the electrode	$\frac{\partial(\epsilon_s c_s)}{\partial t} = \frac{j^{Li}}{F}$
4	Retention of species in the electrolyte	$\epsilon_e \frac{\partial c_e}{\partial t} = D^{eff} \frac{\partial^2 c_e}{\partial x^2} + \frac{1 - t_+^0}{F} j^{Li}$

Nevertheless, due to the intricate interrelation of these equations, all variables manifest both spatial and chronological dimensions [4]. To interpret the equations itemized in Table 1, one must employ numerical techniques, prominently leaning towards Computational Fluid Dynamics (CFD) and leveraging the finite volume technique. The CFD method is inherently an implicit modality, and the inherently nonlinear nature of the governing equations necessitates iterative strategies for solutions. However, these nonlinear equations might induce inconsistency during continuous iterations, thus creating complexities in the resolution procedure. As such, to ensure efficacy with the CFD method, it becomes pivotal to linearize these equations. Post-linearization of the discretized equation system, one can discern a tridiagonal equation system, which is amenable to resolution via the Thomas technique.

## RESULTS AND DISCUSSION

The graph 1 represents the variation in the electrolyte concentration. At the cell's beginning (X=0), the electrolyte concentration starts at its highest, around 2.7 mol/cm<sup>3</sup>. This indicates that, initially, the concentration of ions in the electrolyte is at its maximum, which could be near the anode in many battery designs. As we move along the cell length towards x=0.5 there's a noticeable decrease in the electrolyte concentration. This can be attributed to the ions migrating from the anode to the cathode, resulting in a reduction of ions in the electrolyte in this region.

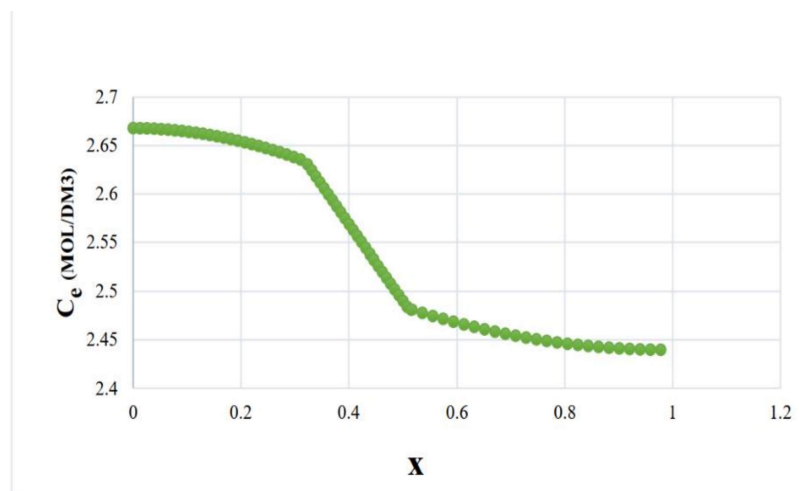


Figure 40: Electrolyte concentration changes profile

Figure 2 visualizes the electrolyte potential distribution along the length of the cell. The continuous and smooth descent signifies that there is a consistent gradient of potential, which could be attributed to the movement of ions, interactions within the electrolyte, and electrode reactions.

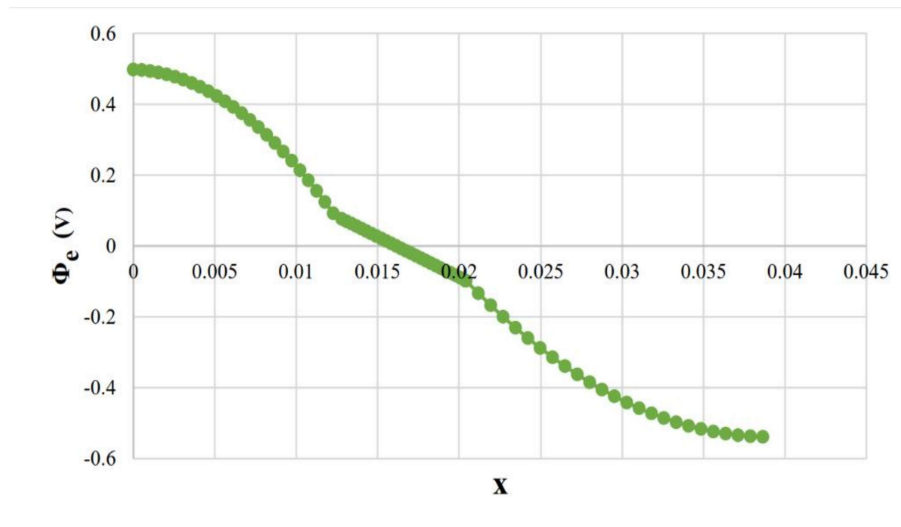


Figure 41: Electrolyte potential changes profile

Figure 3 depicts the electrode potential across the dimensionless length of the cell. The cell's external current arises from the voltage difference between its anode and cathode. Commonly, the potential at the negative electrode is set to zero, making the positive electrode's potential relative to it. Given this basis, the potential at the positive electrode remains consistently elevated in comparison to the surface of the negative electrode.

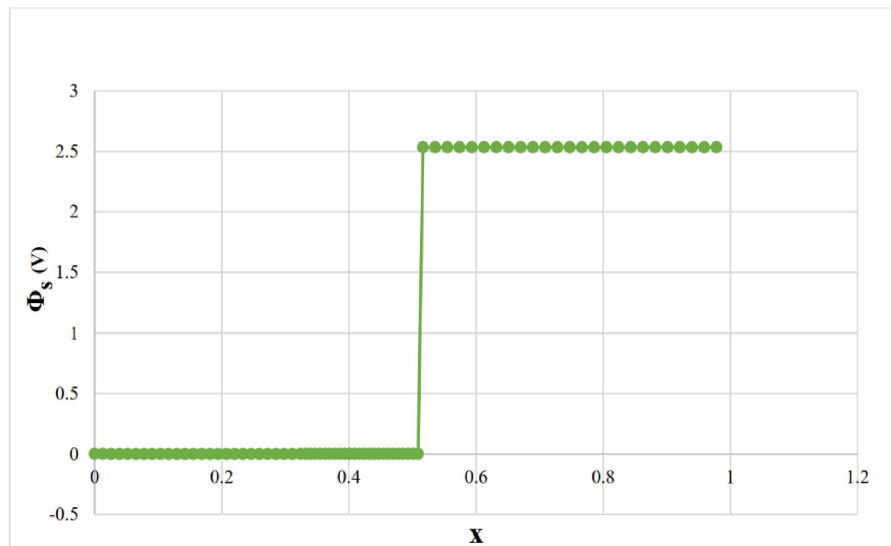


Figure 42: Electrode potential changes profile

Figure 4 offers an in-depth perspective on the electrode concentration across the dimensionless length of the cell during the last 5 minutes of the discharge cycle. The State of Charge (SOC), an essential metric in battery efficacy, displays a marked rise with the passage of time. This time-dependent shift in electrode concentration provides valuable insights into the battery's operational dynamics throughout the discharge period, illuminating the alterations in internal processes and factors with time.

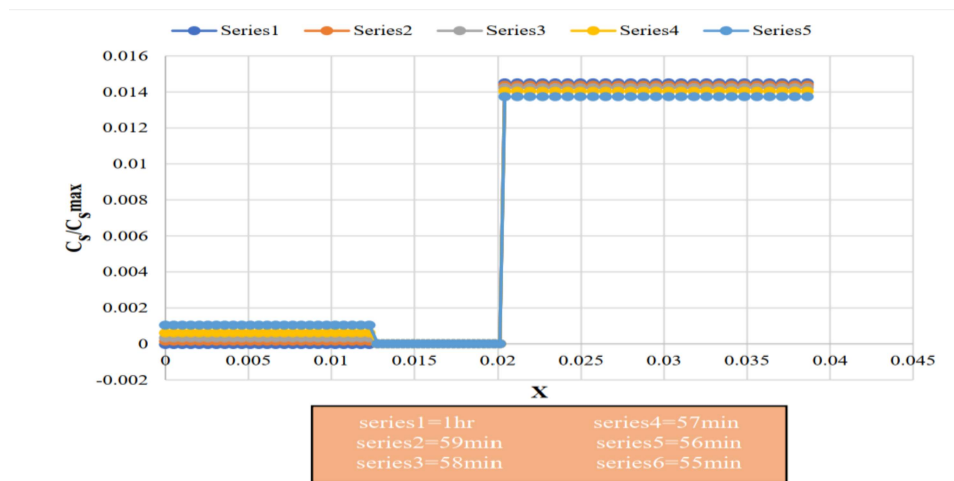


Figure 43: Electrode concentration changes at different times

## CONCLUSIONS

Throughout this research, the unidimensional modeling and simulation approach, combined with the tools of Computational Fluid Dynamics and C++ programming, has been applied to lithium titanate oxide batteries. This methodology has successfully unraveled the intricate equations that dictate the behavior of these batteries. By concurrently evaluating crucial variables, such as electrolyte concentration and electrode potentials, this study has deepened our comprehension of the intricate workings of lithium titanate oxide batteries. This simulation technique serves as an essential tool, especially considering the economic and logistical challenges of experimental tests. As we reflect on the findings, it becomes evident that there is a pressing need for continued exploration and refinement in our modeling approaches. Only through such dedicated efforts can we hope to bridge the gap between the present-day performance of lithium titanate oxide batteries and the potential they hold for future applications.

## REFERENCES

- [1] X. Y. S. Z. a. T. v. R. Yuping Wu, *Lithium-Ion Batteries: Fundamentals and Application*, CRC press, 2015.
- [2] F. W. J. T. L. Y. Naoki Nitta, "Li-ion battery materials: present and future," *Materials Today*, 2015.
- [3] P. A. Farschad Torabi, *Simulation of battery systems: Fundamentals and applications*, Academic Press, 2020.
- [4] F. T. a. A. M. V. Esfahanian, "An innovative computational algorithm," *Journal of Power Sources*, 2008.