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PHYSICS-INFORMED MACHINE LEARNING FOR ELECTRO-THERMAL MODELING
AND HARDWARE-IN-THE-LOOP BATTERY EMULATION

by

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ABSTRACT

The increasing adoption of lithium ion batteries in transportation, maritime power systems, and stationary energy storage applications has created a growing need for accurate electro-thermal battery models capable of supporting system design, validation, and operation. While physical battery testing remains essential, it is often expensive, time intensive, and potentially hazardous, particularly when evaluating new system architectures or extreme operating conditions. As a result, electro-thermal battery modeling and hardware-in-the-loop battery emulation have emerged as valuable tools for reducing development costs while improving testing flexibility and safety.

This work investigates a progression of electro-thermal modeling approaches for real-time battery emulation. The research begins with the development of a physics-based electro-thermal hardware in the loop battery emulator that combines an equivalent circuit model with a reduced order thermal model to reproduce battery voltage and temperature behavior in real time. Building upon this foundation, a deep neural network ensemble is developed to predict voltage, state of charge, and temperature directly from experimental Hybrid Pulse Power Characterization data. While the data driven framework demonstrates the ability to learn complex nonlinear battery behavior, limitations associated with generalization and physical consistency motivate the development of a physics-constrained machine learning approach.

The final study introduces a physics-constrained neural network framework that embeds electro-thermal equivalent circuit relationships and thermal governing equations within the learning process. By combining physically interpretable model struc-

ture with data driven learning, the framework improves model transparency while maintaining the flexibility necessary to capture nonlinear battery behavior. Experimental validation demonstrates accurate prediction of voltage and temperature across dynamic operating conditions while preserving physically meaningful internal states.

Collectively, this work establishes a development pathway from traditional physics based modeling to physics informed machine learning for electro-thermal battery prediction and hardware-in-the-loop emulation. The results demonstrate the potential of hybrid modeling approaches to support future battery emulation platforms, battery management systems, and real time testing environments for advanced energy storage applications.

TABLE OF CONTENTS

ACKNOWLEDGMENTS	ii
ABSTRACT	iii
LIST OF TABLES	vii
LIST OF FIGURES	viii
CHAPTER 1 INTRODUCTION	1
CHAPTER 2 ELECTRO-THERMAL HARDWARE-IN-THE-LOOP BATTERY EM- ULATOR FOR SHIPBOARD SYSTEMS TESTING	6
2.1 Abstract	6
2.2 Introduction	7
2.3 Methodology	9
2.4 Results	15
2.5 Conclusion	17
CHAPTER 3 DEEP NEURAL NETWORK-BASED MODELING OF ELECTRO- THERMAL LITHIUM-ION BATTERIES RESPONSES LEVERAG- ING HYBRID PULSE POWER CHARACTERIZATION	19
3.1 Abstract	19
3.2 Introduction	20
3.3 Methodology	22

3.4	Results	27
3.5	Conclusion	29
CHAPTER 4 PHYSICS-CONSTRAINED NEURAL NETWORKS FOR ELECTRO- THERMAL BATTERY MODELING AND EMULATION		31
4.1	abstract	31
4.2	introduction	32
4.3	Methodology	36
4.4	results	45
4.5	Conclusion	48
CHAPTER 5 CONCLUSION		50
5.1	Conclusion	50
5.2	Challenges	50
5.3	Future Direction	51
BIBLIOGRAPHY		53
APPENDIX A REPRINT PERMISSIONS		58
A.1	Chapter 1: Electro-Thermal Hardware-in-the-Loop Battery Emu- lator for Shipboard Systems Testing	58

LIST OF TABLES

Table 2.1	Tests conducted to build and validate the model.	10
Table 3.1	The amount of HPPC tests run under each condition to collect training data.	26

LIST OF FIGURES

Figure 1.1	The proposed framework for developing or improving a battery model, emulating the battery during controls or hardware design and validation, followed by on-board system implementation.	2
Figure 1.2	A comparison between the required resources, such as time, money, and understanding, to develop each level of battery emulation and their relative benefits.	4
Figure 1.3	The hardware developed for electro-thermal HIL emulation that serves as the foundation for all battery model implementation. . .	5
Figure 2.1	Diagram of the equivalent circuit used in the electrical model. . .	9
Figure 2.2	Thermal circuit used in the reduced order model.	11
Figure 2.3	Diagram of the battery emulator hardware setup.	12
Figure 2.4	The battery emulator hardware setup from (a) the front view and (b) the back view.	13
Figure 2.5	Logical flow to operate the battery emulator.	14
Figure 2.6	The voltage during a) 1C and b) 2C constant current discharges of a K2 26650 LFP cell along with the emulator results for the same cell.	15
Figure 2.7	The temperature during a) 1C and b) 2C constant current discharges of a K2 26650 LFP cell along with the emulator results for the same cell.	16
Figure 3.1	A block diagram to visualize the flow of information through each iteration of a current load profile to predict the electro-thermal response.	22
Figure 3.2	The logical flow to develop and employ the neural network for battery state prediction for a given load profile.	23

Figure 3.3	The voltage throughout an HPPC protocol every 5% state of charge with a closer look at the 80% pulse.	25
Figure 3.4	The experimental setup used to collect HPPC data from three temperature controlled cells simultaneously.	26
Figure 3.5	The a) voltage, b) temperature, and c) state of charge for a load profile as calculated by the model and tested experimentally.	28
Figure 4.1	The process for developing and employing a battery emulator [1] through physics-constrained ML to improve system design and testing of advance shipboard architectures.	35
Figure 4.2	A diagram of the information exchanged between submodels of the electro-thermal physics-constrained ML model.	37
Figure 4.3	A flowchart explaining the training process of the electro-thermal physics-constrained ML battery model.	40
Figure 4.4	The modeled and experimental (a) voltage and (b) temperature across a 4C (12 A) constant current discharge at room temperature ($\sim 23^{\circ}\text{C}$ ambient).	46
Figure 4.5	The modeled and experimental (a) voltage and (b) temperature across an HPPC profile in a 30°C ambient temperature chamber, containing 1C (3 A) pulses every 5% SOC, and C/3 (1 A) discharges between each pulse.	47

CHAPTER 1

INTRODUCTION

The increasing electrification of transportation and energy systems has driven significant growth in the deployment of lithium-ion batteries. Applications ranging from electric vehicles and aircraft to stationary energy storage and shipboard power systems increasingly rely on battery energy storage systems to provide reliable, efficient, and flexible power. As battery systems become more deeply integrated into critical infrastructure, understanding and predicting their behavior has become essential for ensuring safety, performance, and operational reliability.

The behavior of lithium-ion batteries is inherently multi-physical. Electrical performance and thermal behavior are strongly coupled. Temperature affects nearly every aspect of battery operation, including available capacity, power capability, efficiency, degradation rate, and safety. Likewise, electrical loading conditions directly influence heat generation within the cell, causing changes in temperature that subsequently alter electrical performance. As a result, accurate characterization of battery systems requires consideration of both electrical and thermal domains simultaneously.

Experimental testing remains the primary method for evaluating battery performance under realistic operating conditions. However, physical testing presents several challenges. Battery experiments can be time-consuming, costly, and difficult to scale across a wide range of operating scenarios. Furthermore, testing under extreme conditions introduces safety risks associated with overheating, degradation, and thermal runaway. These challenges become increasingly significant when investigating large battery systems or evaluating new system architectures.

To reduce the cost, risk, and time associated with battery development, researchers have increasingly turned toward electro-thermal battery modeling and hardware-in-the-loop (HIL) battery emulation. Electro-thermal models provide a virtual representation of battery behavior that can be used to predict system performance without requiring extensive physical testing. Shown in figure 1.1, when implemented within a hardware-in-the-loop framework, these models can emulate battery behavior in real time, enabling safe and repeatable testing of energy storage systems, power electronics, and control strategies. Therefore, the development of accurate and computationally efficient electro-thermal battery models is a critical step toward advancing battery system design, validation, and deployment.

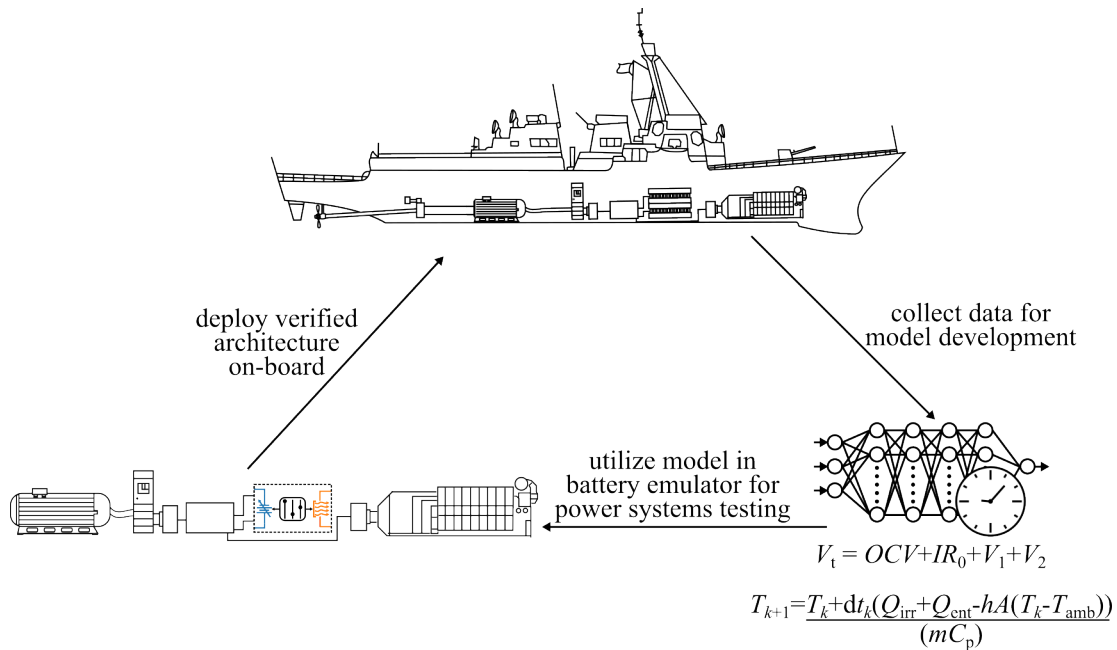


Figure 1.1 The proposed framework for developing or improving a battery model, emulating the battery during controls or hardware design and validation, followed by on-board system implementation.

The effectiveness of electro-thermal battery emulation depends heavily on the underlying battery model. To be useful in real-time applications, battery models must satisfy several competing requirements. They must accurately reproduce the electrical and thermal response of a battery under varying operating conditions while remaining

computationally efficient enough for real-time execution. Additionally, they should generalize across a range of temperatures, loading conditions, and operating states while maintaining physical consistency with known battery behavior.

Traditional reduced-order physics-based models have been widely adopted because they provide a balance between accuracy and computational efficiency. Equivalent circuit models coupled with reduced-order thermal models can be implemented in real time and are well suited for battery management and emulation applications. However, these approaches often require extensive parameterization and may struggle to fully capture highly nonlinear battery dynamics across diverse operating conditions.

Recent advances in machine learning have created new opportunities for battery modeling. Data-driven approaches can learn complex nonlinear relationships directly from experimental data and often require less manual model development. Neural networks and other machine learning methods have demonstrated promising results for predicting battery voltage, temperature, and state variables. Nevertheless, purely data-driven methods introduce new challenges. Their performance depends heavily on training data quality and coverage, they may extrapolate poorly beyond observed operating conditions, and they often lack the physical interpretability and consistency desirable for engineering applications.

Consequently, a gap exists between traditional physics-based modeling approaches and modern data-driven methods. The central problem addressed by this thesis is how to develop electro-thermal battery models that balance fidelity, computational efficiency, adaptability, and physical interpretability while remaining suitable for real-time hardware-in-the-loop battery emulation.

The objective of this thesis is to develop and evaluate electro-thermal battery modeling approaches that support real-time emulation, with the goal of enabling safer, lower-cost, and more flexible testing of battery-powered systems without relying exclusively on physical batteries.

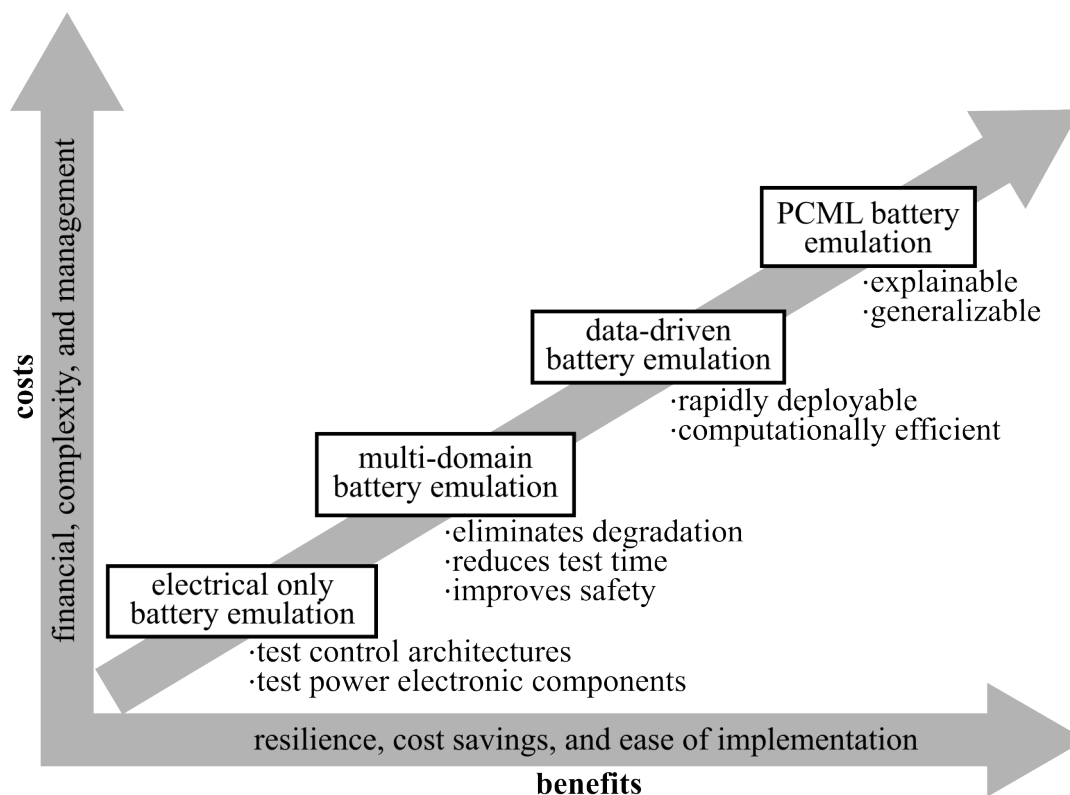


Figure 1.2 A comparison between the required resources, such as time, money, and understanding, to develop each level of battery emulation and their relative benefits.

To accomplish this objective, the research presented in this thesis investigates a progression of modeling approaches that span the spectrum from traditional physics-based methods to modern machine learning techniques, seen in figure 1.2. The first study focuses on the development of a physics-based electro-thermal hardware-in-the-loop battery emulator capable of reproducing both electrical and thermal battery behavior in real time, the hardware of which is shown in figure 1.3. Building upon this foundation, the second study explores a fully data-driven approach using deep neural networks to predict battery electro-thermal response from experimental characterization data. Finally, the third study introduces a physics-informed machine learning framework that combines the physical structure of traditional battery models with the adaptability and predictive capability of machine learning.

Together, these studies seek to identify modeling approaches capable of supporting

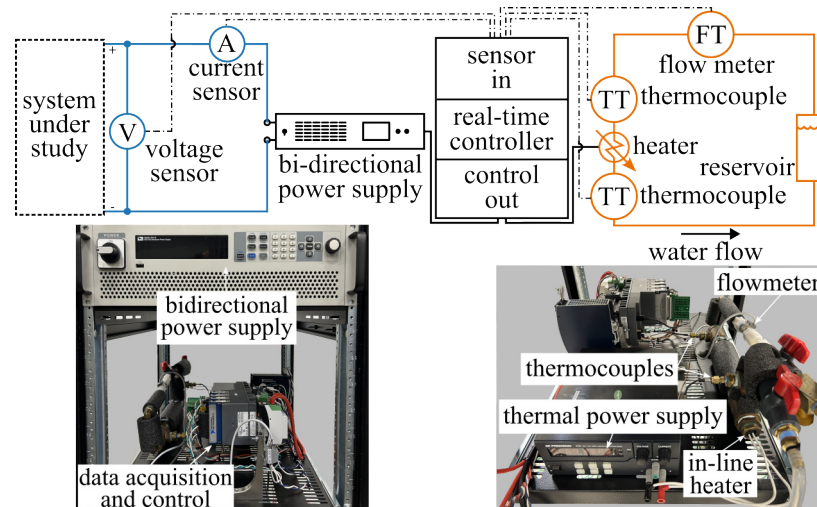


Figure 1.3 The hardware developed for electro-thermal HIL emulation that serves as the foundation for all battery model implementation.

next-generation electro-thermal battery emulation systems.

This work focuses on electro-thermal modeling of lithium-ion batteries at the cell level. Particular emphasis is placed on predicting voltage, state of charge, and temperature behavior using experimentally derived battery characterization data. The research considers modeling approaches suitable for real-time implementation and battery emulation applications.

The work presented herein does not seek to fully address all aspects of battery system design. Topics such as battery aging, degradation modeling, advanced battery management system development, and large-scale pack-level implementation are beyond the scope of this thesis. While these areas are important extensions of electro-thermal battery modeling, they are reserved for future investigation.

CHAPTER 2

ELECTRO-THERMAL HARDWARE-IN-THE-LOOP BATTERY EMULATOR FOR SHIPBOARD SYSTEMS TESTING

This chapter is wholly based on “Electro-thermal Hardware-in-the-Loop Battery Emulator for Shipboard Systems Testing,” accepted for publication in the IEEE ESTS 2025 Conference Proceedings [1].

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2.1 ABSTRACT

The transition to all-electric marine vessels has elevated the importance of batteries in meeting high-pulsed loads and efficiency requirements. Understanding the electrical and thermal responses is vital to both safety and cost in battery energy storage system development. To address this, an electro-thermal hardware-in-the-loop (HIL)

battery emulator has been developed, integrating a bi-directional power supply and a cooling loop heater to replicate both electrical and thermal behaviors. The output for each is determined by a real-time controller running a coupled electrical and thermal model, based on an equivalent circuit and a reduced-order model, respectively. The parameters for model operation are determined by cell testing and curve fitting. This work seeks to define an approach for characterizing any lithium-ion battery for a given energy storage system, and presents progress on the hardware that comprises the emulator. The ability to substitute the battery in a testbed while evaluating its effectiveness, especially in edge-case scenarios, significantly reduces hazards and costs when determining the right battery. Using a lithium iron phosphate 26650 cell as a case study, this work demonstrates the accuracy of this method, emulating the voltage and temperature of a 1C constant current discharge with an average error of 1.14% and 0.89%, respectively. At 2C, the voltage emulation error was found to be 2.07% and the temperature error was found to be 1.39%.

2.2 INTRODUCTION

Evident by the recent push for electrification of transportation, tactical energy management has become a priority in all sectors. As seafaring travel accounts for 90% of transoceanic trade, hybrid and all-electric ships are the expected next steps for the global shipping industry, with General Electric and Siemens having already completed all-electric propulsion systems [2, 3]. Frequently requiring variable operation states of shipboard power systems, Battery Energy Storage Systems are essential for ensuring stable microgrid operation [4]. However, testing lithium-ion batteries, an onboard energy storage system of great interest, quickly becomes expensive and dangerous when examining new system architectures. A hardware-in-the-loop substitute for these batteries provides a safer and more sustainable alternative for investigating battery chemistries, cooling strategies, and Battery Management Systems [5]. Exist-

ing research on a multi-domain battery emulation often neglects thermal emulation beyond its affect on electrical parameters [6]. While electrical-only emulation can determine voltage, state of charge (SOC), and remaining useful life from an external load, it does not account for heat generation. However, as current increases, Ohmic heating becomes a significant factor [7]. This is relevant for all-electric ships, where rapidly shifting loads can require batteries to supply up to 70% of the total microgrid power needs at a given time. To ensure safe and efficient system operation, battery thermal response must be integrated into the system architecture [4].

Lithium-ion batteries encompass a wide array of chemistries tailored for different priorities including safety, energy density, and cost. Lithium Iron Phosphate (LFP), the chemistry used in this study, is known for superior thermal stability and cycle life, at the cost of lower energy density compared to nickel manganese cobalt (NMC) or nickel cobalt aluminum (NCA) chemistries [8]. NMC and NCA offer higher energy density, making them attractive for weight constrained energy storage, but require strick thermal management due to lower thermal runaway thresholds. Emerging chemistries such as lithium sulfur, or solid state batteries are gaining interest for their higher theoretical capacity, or safety potential, but are not technologically ready for application [9].

Naval platforms present unique challenges for battery systems, including high-power pulse loads from systems such as railguns, radar arrays, and directed energy weapons [10]. These applications demand batteries that can handle large transient currents while maintaining thermal and electrical stability. Real-time emulation becomes critical for testing such scenarios safely. Hardware-in-the-loop (HIL) setups allow for the validation fo control systems, thermal responses, and power system design without the cost of destructive testing [11]. Additionally, HIL emulators can support fault injection and abuse scenario testing that would be unsafe with physical packs.

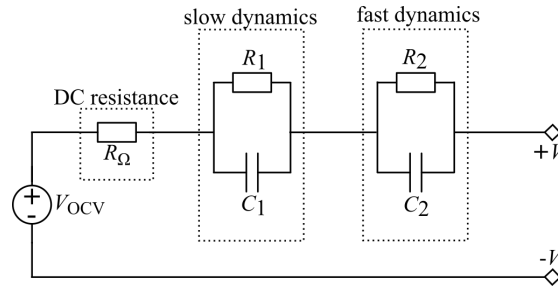


Figure 2.1 Diagram of the equivalent circuit used in the electrical model.

Electro-thermal battery emulation offers a potential to test and validate both the electrical and thermal aspects of a battery in connection with the electro-thermal design and development of power systems. To expand, the proposed electro-thermal battery emulator is designed to replicate both the heat generated into a liquid cooling system, and the electrical response of the desired battery. In previous work, Peskar et al. [12] introduced a foundational framework for developing an electro-thermal battery emulator and presented preliminary results emulating a 18650 3.6 V 3 Ah lithium nickel cobalt aluminum oxide (NCA) cell. In this work, progress on the development of an emulation system methodology and supporting hardware is presented. The contributions of this work are twofold. First, it examines the electro-thermal simulation of a more modern cell geometry and chemistry, using a 26650 3.2 V 2.6 Ah Lithium iron phosphate (LFP) cell. Second, it provides an update on the physical hardware that makes up the emulator and reports the results obtained from experimental validation.

2.3 METHODOLOGY

2.3.1 ELECTRICAL MODEL

The coupled electro-thermo model can be separated into two subsystems that share parameters, and will be referred to as the electrical and thermal models. The electrical model updates the voltage, open-circuit voltage (OCV), current across the battery, and the SOC. As shown in Fig. 2.1, the electrical response is modeled as

Table 2.1 Tests conducted to build and validate the model.

data collection	purpose
HPPC at $T_{\min}$ and $T_{\max}$	fitting R_{Ω} , R_1 , R_2 , C_1 , C_2
C/10 CC at $T_{\min}$ and $T_{\max}$	estimate OCV
1C CC discharge	validation data
2C CC discharge	validation data

a second-order equivalent circuit, which was selected for its balance between fidelity and computational efficiency. The equivalent circuit relies on six parameters, the open circuit voltage of the battery, the DC internal resistance, and two resistance and capacitance pairs that capture the battery dynamics. These parameters are implemented through lookup tables dependent on the SOC, temperature, and current loading (C-rate) of the cell. To build the necessary lookup tables, the required experimental data is summarized in Table 3.1. Although this work uses an LFP cell as a case study, the proposed electro-thermal emulation architecture is extendable to other lithium-ion chemistries and beyond, whether that be lithium nickel manganese cobalt oxide (NMC), or even solid-state cells. Emulating another chemistry would require reparameterization of the lookup tables derived through HPPC and OCV testing, as summarized in Table 3.1.

The DC internal resistance and battery dynamics can be determined using Hybrid Pulse Power Characterization (HPPC) at the minimum and maximum expected operating temperatures. HPPC is a standard method for evaluating the dynamic performance of a battery [13]. This is done by analyzing the battery's response to discharge pulses at specific SOC and temperatures. The resistances and capacitances defining the battery dynamics can then be found using nonlinear least squares fitting. The OCV can be estimated and fitted from constant current (CC) C/10 discharges

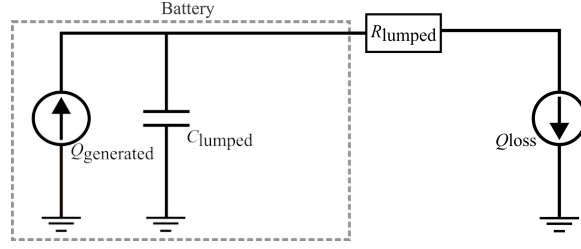


Figure 2.2 Thermal circuit used in the reduced order model.

at each edge of the temperature range. Once obtained, these parameters can be validated against moderate rate discharge data at varying temperatures. While additional data can increase modeling accuracy, the tests outlined in Table 3.1 represent the minimal requirements for emulator operation.

$$V_{\text{terminal}}(t) = V_{\text{OCV}}(\text{SOC}, T) - V_1(t) - V_2(t) - I(t) * R_{\Omega}(\text{SOC}, T, C_{\text{rate}}) \quad (2.1)$$

The equivalent circuit is defined by equation 2.1, which describes the battery voltage as a function of time [14]. The OCV and DC internal resistance dependent on the SOC and temperature, and they are updated at each iteration by the electrical and thermal models, respectively.

$$V_i(t) = \alpha_i * V_{i,t-1} + R_i(\text{SOC}, T, C_{\text{rate}}) * (1 - \alpha_i) * I(t) \quad (2.2)$$

$$\alpha_i = e^{-\Delta t * R_i * C_i} \quad (2.3)$$

Equation 2.2 defines V_1 and V_2 , which are used in equation 2.1. These voltages account for the battery dynamics and are updated at each iteration based on α_i as described by equation 2.3. Similar to the DC internal resistance, the dynamic resistance and capacitance vary with SOC, temperature, and discharge rate.

2.3.2 THERMAL MODEL

The thermal model, defined by equation 2.4, calculates the heat generated and dissipated to update the cell temperature. The heat transfer model, as shown in Fig. 2.2,

is a lumped thermal circuit, and employs the isothermal reduced-order heat generation model, described by equation 2.5, which assumes uniform heat generation. The heat transfer model relies on two lumped parameters. C_{lumped} represents the total thermal mass, which is the product of the cell mass and heat capacity, and R_{lumped} represent the total thermal resistance from the cell to ambient air.

$$T(t) = T(t-1) + \left(\left(-\frac{1}{C_{\text{lumped}} * R_{\text{lumped}}} \right) * T(t-1) + \left(\frac{1}{C_{\text{lumped}} * R_{\text{lumped}}} \right) * T_{\infty} + \left(\frac{Q_{\text{gen}}}{C_{\text{lumped}}} \right) \right) * \Delta t \quad (2.4)$$

$$Q_{\text{gen}} = I(t) * \left(V_{\text{OCV}}(\text{SOC}, T) - V_{\text{terminal}}(t) \right) + I(t) * \frac{du}{dT} \quad (2.5)$$

Equation 2.5 describes heat generation within the cell as the difference between OCV and voltage at the terminals multiplied by the discharge current [15]. The OCV and terminal voltage being shared by the electrical model. Additionally, entropy is accounted for as the current multiplied by the rate of change of OCV with respect to temperature. However, accurately determining the entropy contribution requires specialized experimental procedures, which were beyond the scope of this study and were thus neglected.

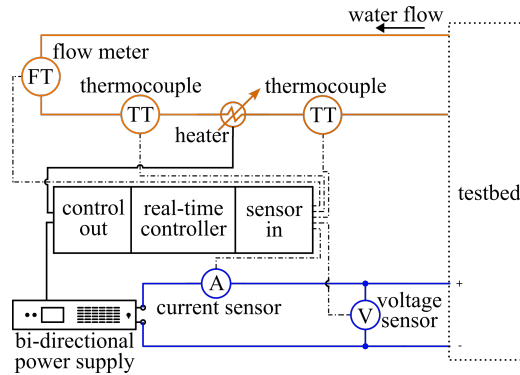


Figure 2.3 Diagram of the battery emulator hardware setup.

2.3.3 HARDWARE-IN-THE-LOOP

Figure 2.3 highlights the connections within the battery emulator hardware. The model, running on the real-time controller, couples the separate electrical and thermal domains. The controller receives real-time updates on heat dissipation via a flow transducer and two temperature transducers in the cooling loop, and collects electrical measurements using voltage and current sensors. The emulator cooling loop is connected to a pump submerged in a tank, and the bi-directional power supply interfaces with an electronic load. This setup allows the emulator to be connected to a microgrid testbed by swapping out the electronic load and cooling tank as needed.

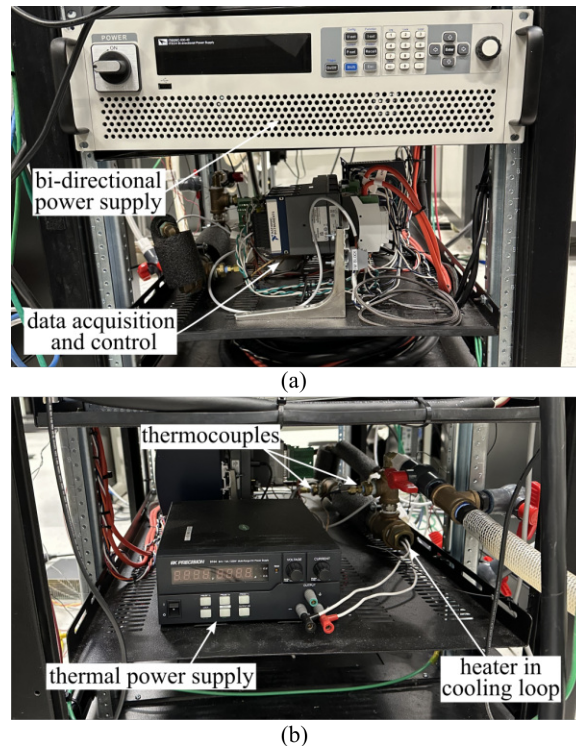


Figure 2.4 The battery emulator hardware setup from (a) the front view and (b) the back view.

Figure 2.4 shows the implementation of the hardware-in-the-loop emulator, employing a bi-directional power supply (IT6000C-500-40) for electrical emulation and an analog power supply (BK 9104) heating a cooling loop. Both power supplies are controlled by a cRIO-9054 from NI, which runs the model at 100 Hz, and adjusts the

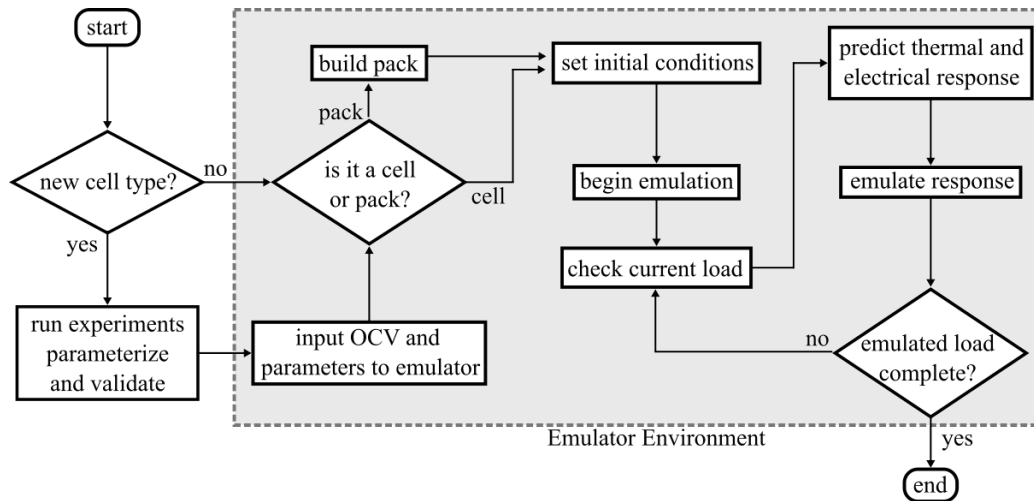


Figure 2.5 Logical flow to operate the battery emulator.

outputs of each power supply accordingly.

2.3.4 USAGE PROCEDURE

Figure 2.5 demonstrates the process of using the battery emulator to test any lithium-ion battery. If the cell is not a new type, whether in terms of chemistry, size, or brand, and the test is not conducted at the pack level, the emulator only requires initial conditions for operation. If given a new pack layout or when moving from a cell to a pack level, the series and parallel configuration must be defined in the software to allow the emulator to scale its outputs accordingly. Once the pack is configured, the emulation can proceed the provided initial conditions. This capability is particularly useful for large battery packs, such as those used in all-electric ships, where high power demands and significant heat generation make physical testing both costly and hazardous. The emulator offers a safer and more cost-effective alternative. While this emulates average pack behavior, it does not yet model inter-cell thermal interactions or imbalance.

In the case of a new cell type, there are steps outside of the emulator environment that must be completed first. Cell testing is required to collect data and determine the model parameters, completing at minimum those listed in Table 3.1. The model

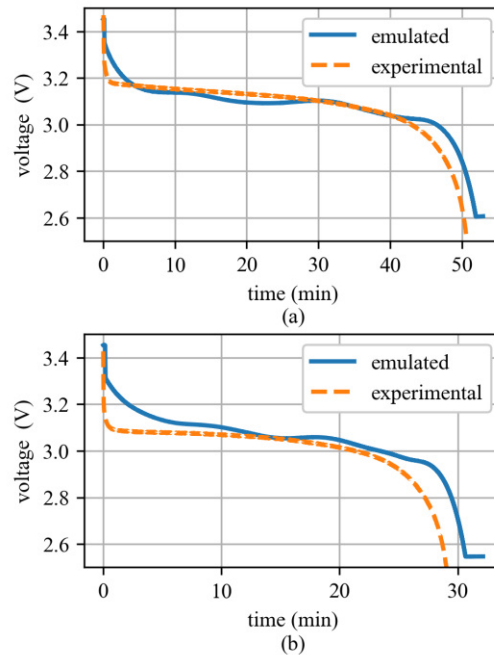


Figure 2.6 The voltage during a) 1C and b) 2C constant current discharges of a K2 26650 LFP cell along with the emulator results for the same cell.

must then be updated with the new parameters and data, and should be validated against moderate rate tests. Once this process is complete, the emulator environment can then be used to test the cell or pack under a load, limited only by hardware.

2.4 RESULTS

Reported in figures 2.6 and 2.7, the performance of the emulator was evaluated relative to the physical counterpart for a K2 Energy 26650 lithium iron phosphate battery under 1C and 2C constant current discharge conditions. Previously used in a naval railgun, the 2.6Ah cells used were developed for high power pulsed loads, and were expected to perform well under the 2C test. The 1C shows that the emulator could emulate the voltage with 1.14% average error and the temperature with 0.89% average error. This demonstrates that both the model and hardware of the emulator could replicate the dynamics of the cell at 1C. At 2C, the error increased, yet remained within acceptable bounds for early-stage HIL testing, with the voltage emulation er-

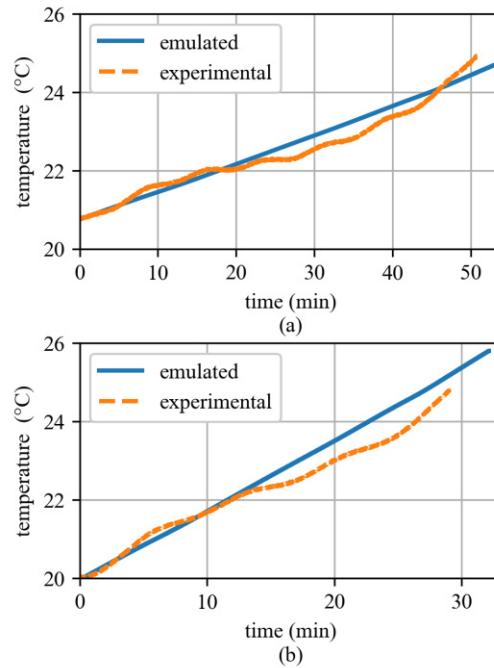


Figure 2.7 The temperature during a) 1C and b) 2C constant current discharges of a K2 26650 LFP cell along with the emulator results for the same cell.

ror reaching 2.07% and temperature was found to be 1.39%. However, further model development is required for applications exceeding 2C.

The increase in error for the test conducted at 2C was expected due to the neglected entropic ($\frac{dU}{dT}$) heat generation mode. At C-rates higher than 1C, the internal reaction rates are known to increase, causing more dynamic temperature variation due to the larger contribution of the entropy. This effect explains the higher variance seen in the 2C test. Future versions will seek to account for entropic heating via data driven methods to improve high-rate fidelity. However, the overall trend of increasing temperature was still well captured as the maximum variance was remaining within $\pm 1^\circ\text{C}$. Further contributions to the total error seen in both the 1C and 2C tests is derived from modeling assumptions and the use of averaged values. The tested K2 26650 batteries were not new cells and had an unknown history, leading to an unknown state of health. This uncertainty complicated parameterization and testing of the cells as the calculated parameters varied across each cell tested. This variance

from the cells leads to uncertainty in electrical parameters as they might fit well for one cell but inaccurate for another. Using new cells or cells with a documented history is imperative for obtaining more certain parameters that accurately represent the cell and its current state.

2.5 CONCLUSION

To meet the demands of all-electric ships, a hardware-in-the-loop battery emulator is needed to safely test the electrical and thermal characteristics of lithium-ion batteries. This work demonstrated the capabilities of a hardware-in-the-loop battery emulator assessed on the accuracy of replicating electrical and thermal responses under moderate constant current discharge rates. Using a second order equivalent electrical circuit and a reduced-order thermal model, a cRIO-9054 is used to control a bi-directional power supply and an analog power supply to emulate the electrical and thermal output of a K2 26650 lithium iron phosphate cell. The emulator was able to produce a temperature response with 0.89% and 1.39% average error at 1C and 2C, respectively, while the voltage response average error was 1.14% at 1C and 2.07% at 2C.

Future work will explore advanced model development to support high C-rate loads and irregular temperatures. However, continued work to understand cell degradation and improve modeling accuracy is needed and will provide insight on the true parameters of the cells, once state of health reference points are obtained. Investigation of scaling factors and pack design will allow pack level emulation from single cell characterization, to provide safer testing of high voltage and high power battery packs, as used in commercial systems. Pack-level emulation also introduces challenges including cell to cell variability, unequal thermal loading, and BMS response under fault conditions, all of which will be targets of future model refinement.

Integrated into a full testbed, a coupled electro-thermal battery emulator could

serve applications beyond determining battery selection. A single emulator can provide insights on the rapid development of a battery management system for both electrical and thermal control. Additionally, multiple emulators could be deployed to facilitate the design of battery control systems across multiple packs. Because the initial SOC of the battery is a set parameter, the time investment for testing these systems will be greatly reduced since the emulator does not recharging, only reinitialization. Removing a real battery from a system allows harsher, safer, and more thorough testing than previously possible.

ACKNOWLEDGMENT

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CHAPTER 3

DEEP NEURAL NETWORK-BASED MODELING OF ELECTRO-THERMAL LITHIUM-ION BATTERIES RESPONSES LEVERAGING HYBRID PULSE POWER CHARACTERIZATION

This chapter is wholly based on “Deep Neural Network-based Modeling of Electro-thermal Lithium-ion Batteries Responses leveraging Hybrid Pulse Power Characterization,” accepted for publication in ASME IMECE conference, 2025 [16].

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3.1 ABSTRACT

Predicting the electro-thermal response of lithium-ion batteries is critical for energy storage system integration. However, due to their rate dependent behavior battery testing is expensive and time intensive. There is a need to develop reliable predic-

tive models that can emulate the electro-thermal behavior of a battery. Traditional physics-based models, while effective, are computationally intensive and require detailed knowledge of electro-chemical properties to parameterize, making them difficult to implement for hardware-in-the-loop battery system testing. To address these limitations, this paper presents a data-driven electro-thermal battery modeling approach using deep neural networks trained on hybrid pulse power characterization data. The proposed model aims to predict both electrical and thermal responses of lithium-ion batteries under various dynamic load conditions, offering a scalable and efficient alternative to physics-based electro-thermal battery modeling. Applying an iterative approach to step through a load profile, a deep neural network ensemble predicts the change in temperature, voltage, and state of charge given previous conditions was able to calculate future behavior for a 1C constant current discharge with 0.07 V, 2.35%, and 0.25°C average absolute error, for voltage, state of charge, and temperature respectively.

3.2 INTRODUCTION

Operational and maintenance costs are critical concerns for the maritime industry. Ships often face high maintenance cost due to power fluctuations that degrade engine performance and increase wear. To address these inefficiencies, the integration of energy storage systems has been investigated as a means to smooth load fluctuations and enable engines to operate closer to their optimal efficiency [17]. These benefits have driven growing interest in the continued electrification of shipboard power systems. Due to the nature of the maritime industry, electrification requires the application of efficient and robust mobile energy storage systems. To validate these systems at the design stage, battery emulators are often used [5]. Interest in electro-thermal battery emulation systems [12] is growing, as they enable more efficient electro-thermal testing and deployment of energy storage systems. This work develops data-driven

models that could be leveraged by electro-thermal battery emulators in the future.

Owing to their high energy density, long cycle life, and falling cost, the deployment of lithium-ion batteries has surged [18]. However, significant challenges arise surrounding battery misuse, including overheating, deep discharging, and thermal runaway [19]. These issues pose a major risk to lithium-ion battery's implementation on maritime platforms. To improve robustness, accurate electro-thermal modeling and prediction of battery behavior are imperative before degradation or safety hazards occur [20]. Physics-based models, such as the equivalent circuit model or the single particle model, require extensive computation and are difficult to implement due to the nonlinear behavior of batteries [21].

The subsequent rise in data-driven methods has highlighted neural networks for capturing the nonlinear dynamics subject to a wide array of variables [22]. While the electrical and thermal domains within a battery are highly interdependent, existing research employing neural networks for battery prognostics has seen success in both domains, regarding state of charge (SOC) [23] and temperature estimation under varying conditions [24]. Furthermore, neural networks significantly reduce the cost of computation, a major limitation in the application of physics-based models [25], enabling real-time monitoring of the dynamics that complex physics-based models could not previously support.

This work introduces a framework for developing and employing deep neural network ensemble (DNNE) to predict the electro-thermal response of a lithium-ion battery via hybrid pulse power characterization (HPPC). To expand, the proposed electro-thermal model will employ a group of neural networks to estimate the change in voltage, state of charge, and temperature as a response to a current to calculate the battery state under the considered load profile. The contributions of this paper are twofold. First, it illustrates the development of a deep multi-layer perceptron ensemble for predicting battery behavior in multiple domains, demonstrating a data-

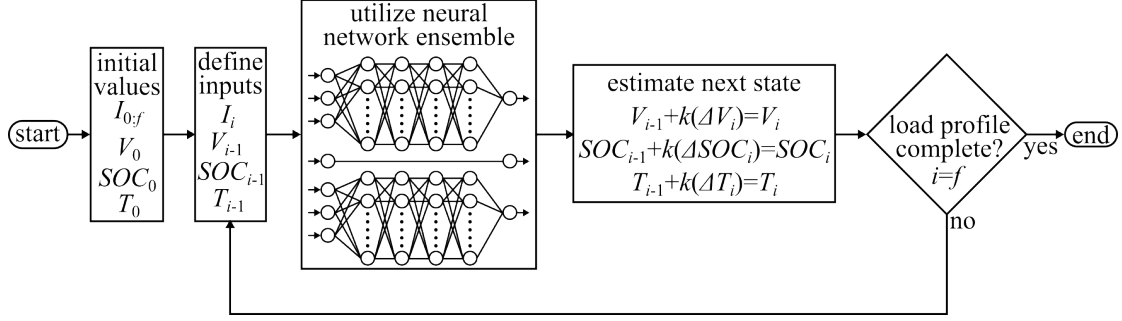


Figure 3.1 A block diagram to visualize the flow of information through each iteration of a current load profile to predict the electro-thermal response.

driven method to minimize cost of computation for complex nonlinear relationships. Second, it builds the groundwork for a robust data collection method utilizing HPPC to allow a wide range of model applicability.

3.3 METHODOLOGY

This section introduces the proposed DNNE and supporting testing and training methodologies.

3.3.1 DEEP NEURAL NETWORK ENSEMBLE

The deployment of the DNNE to predict battery state throughout a load profile is outlined in figure 3.1. Requiring the initial voltage, state of charge, temperature, and scheduled applied current, the model determines the expected change in each variable to predict the next state. Having been trained on data of ten second windows, the predicted change in state is over the next ten seconds of operation, requiring a scaling factor (k), proportional to the step change in time (Δt), as seen in equation 3.1. Iterating through, after the initial values are used to predict the first state under load, the input to the model is replaced by the most recent predicted state for each step

$$k = \frac{\Delta t}{10}. \quad (3.1)$$

From development to implementation, the process to utilize a DNNE to predict the battery state for a load profile via HPPC training is represented in figure 3.2. While data collection is time intensive up front, HPPC under varied conditions provides a strong foundation for learning. To minimize tuning efforts, all three submodels were trained using the Adam Optimizer [26].

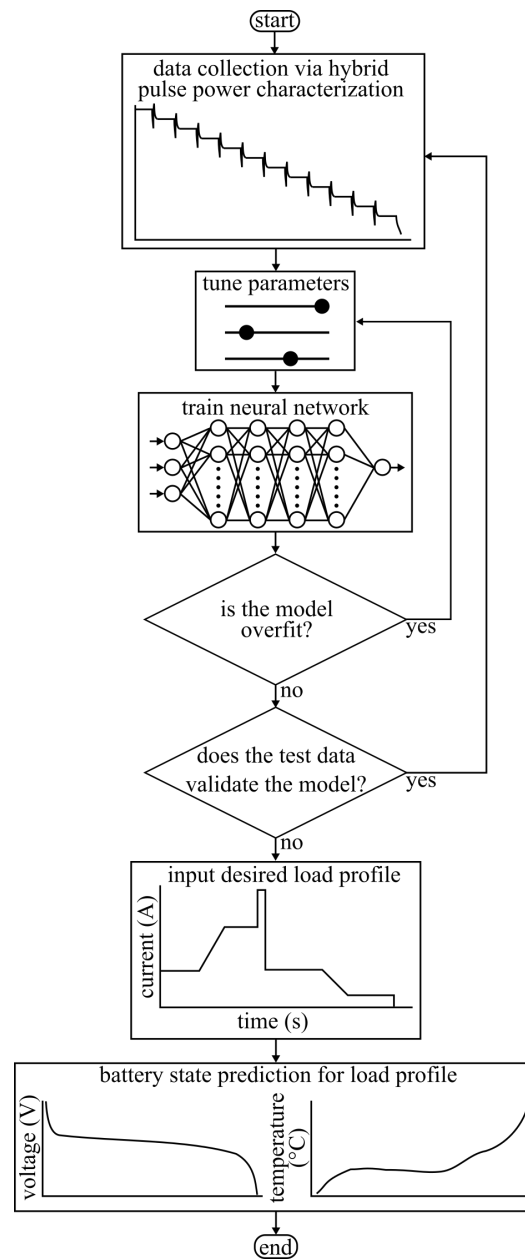


Figure 3.2 The logical flow to develop and employ the neural network for battery state prediction for a given load profile.

To learn and predict complex nonlinear battery characteristics, rather than a single multiple output neural network, an ensemble of parallel networks was chosen. Separating each model mitigates overfitting to HPPC training [27], and increases resilience to noise as well as unexpected input outliers [28]. Comprised of three submodels, one for each output, the DNNE requires four inputs: current (I_i), previous voltage (V_{i-1}), previous SOC (SOC_{i-1}), and previous temperature (T_{i-1}), to predict the change in voltage (ΔV_i), change in state of charge (ΔSOC_i), and change in temperature (ΔT_i), for each step. Including four hidden layers, each containing twenty nodes, the input layer of voltage step submodel receives the current, previous voltage, and previous SOC. Similarly, the submodel to predict the change in temperature is a deep neural network; however, it contains three hidden layers, including 10, 10, and 9 neurons each. The temperature submodel has an input layer requiring the current, previous SOC, and previous temperature. Both deep neural networks make use of the rectified linear unit as the activation function to introduce nonlinear relationships between the data, while mitigating the vanishing gradient problem [29]. Alternatively, the network used to predict the change in state of charge only receives current information. Due to the linear nature of SOC, no hidden layers were used but is left in the form of a neural network for consistency.

The batch size and learning rate are key in avoiding over-generalization and overfitting [30], so the models should be tuned against constant current test conditions as HPPC training often highlights dynamic behavior. Once the model is validated, the DNNE can be employed to instantly predict the battery state over long term load applications.

3.3.2 HYBRID PULSE POWER CHARACTERIZATION

In this work, HPPC is used to extract the response from an 18650 3.6V 3000 mAh lithium nickel manganese cobalt (NMC) cell (Samsung 30Q). HPPC is a protocol

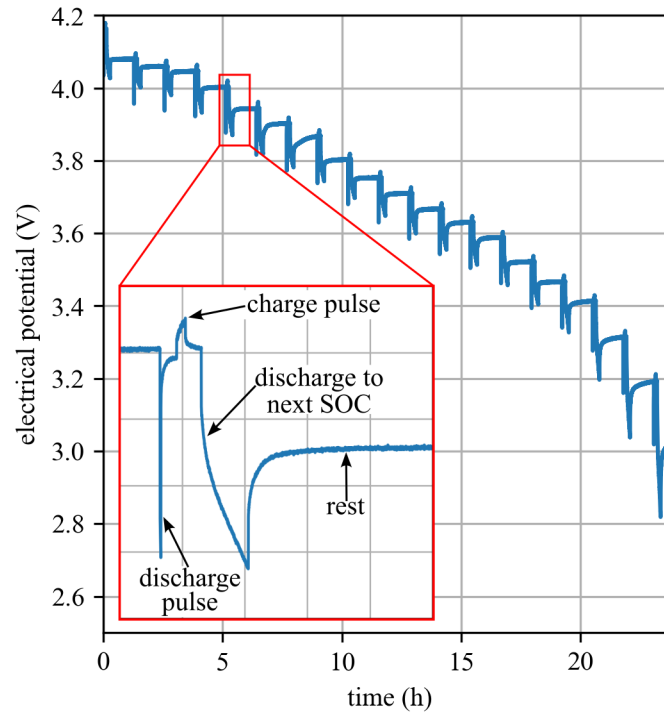


Figure 3.3 The voltage throughout an HPPC protocol every 5% state of charge with a closer look at the 80% pulse.

frequently used to build physics-based models for its ability to highlight the dynamic characteristics a battery exhibits under load [31]. Shown in figure 4.5, the HPPC protocol conducts a discharge and charge pulse at every 5% SOC. Prior to each HPPC test the cells were charged under a constant current $0.5C$, followed by a constant voltage until the current was less than $0.05C$; therefore, it can be assumed that each protocol was started from 100% SOC. From the discharge pulse, rate constants can be determined for a physics-based equivalent circuit model. Developing a data-driven model, this discharge schedule allows the DNNE to learn the dynamic behavior without requiring extensive computation of electro-chemical equations.

Monitoring the battery response to HPPC protocol was conducted using the experimental setup displayed in figure 3.4. To observe the thermal response, each cell had a thermocouple placed on the outer center of the cell case using an NI-9210 thermocouple single conditioner at 1 S/s. Electrical data acquisition and control is

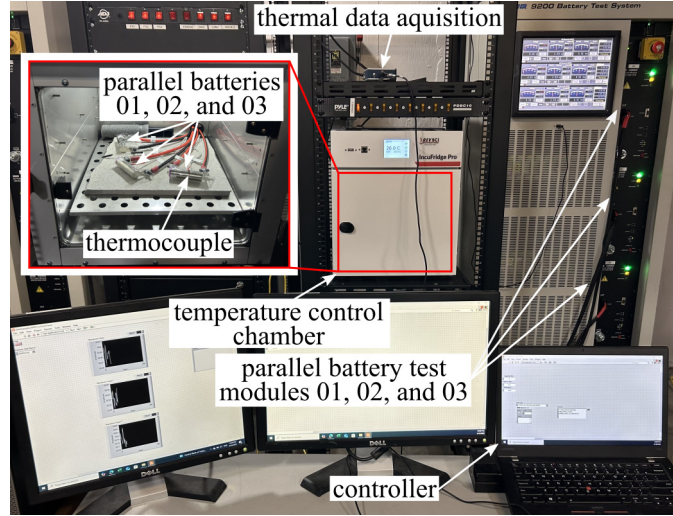


Figure 3.4 The experimental setup used to collect HPPC data from three temperature controlled cells simultaneously.

conducted through the NHR-9200 battery tester also at 1 S/s. A sampling rate of 1 Hz was chosen to minimize the effect noise might have during model training, which was further decreased to 0.1 Hz during data processing. As outlined in table 3.1, HPPC data was collected from three different cells at three pulse rates of 0.5C, 1C, and 2C, and at three ambient temperatures of 20°C, 30°C, and 40°C, using an IncuFridge Pro temperature control chamber. Variable rate and temperature data was necessary for each neural network to autonomously learn the complex relationships between the electrical and thermal parameters in order to build a robust model capable of generalizing to different load conditions as

$$SOC(i) = SOC_{i-1} - \frac{1}{Q_{nom}} \int (I(t)dt). \quad (3.2)$$

Table 3.1 The amount of HPPC tests run under each condition to collect training data.

	discharge pulse rate		
T_{amb}	C/2	1C	2C
20°C	3	3	3
30°C	3	3	3
40°C	3	3	3

3.3.3 TRAINING THE DEEP NEURAL NETWORK ENSEMBLE

Raw data contains current, voltage, and temperature data for each battery, so significant data processing is necessary before the neural network can be trained. State of charge at each step ($SOC(i)$) was calculated via coulomb counting, described by equation 3.2, where the current ($I(t)$) was integrated over each step, then normalized by the nominal capacity (Q_{nom}). To determine the change in SOC, the normalized capacity is then subtracted from the previous state of charge (SOC_{i-1}). Because each neural network requires target outputs for training, the change in voltage, state of charge, and temperature for each step was then appended. Each model was developed using the MLPRegressor function from the scikit-learn python library, requiring the data be scrubbed for errors in acquisition such as missing, or infinite values due to toolkit sensitivities. As the DNNE is not time oriented, all of the data is appended to one file, and used for either training or validation; however, data collected at 1 Hz proved too noisy for learning. Windowing the data into 10 s frames prevented errors due to noise, yet was fast enough to retain the dynamic behavior of the battery. For each 10 s frame, the average current, initial voltage, initial SOC, and initial temperature were input to the model, and it was trained to output the difference in voltage, SOC, and temperature. Moreover, frames that contained an average current of greater than -0.9 A were not used in training, due to voltage relaxation after a discharge producing a positive change in voltage despite a negative average current.

3.4 RESULTS

The model showed good agreement between the DNNE and a Samsung 30Q 18650 lithium nickel manganese cobalt cell under a 1C constant current discharge as reported in figure 3.5. Under a 1C discharge, the average absolute error in voltage, state of charge, and temperature prediction was 0.07 V, 2.35%, and 0.25°C, respectively. The error in voltage and temperature can be attributed to two primary factors. First,

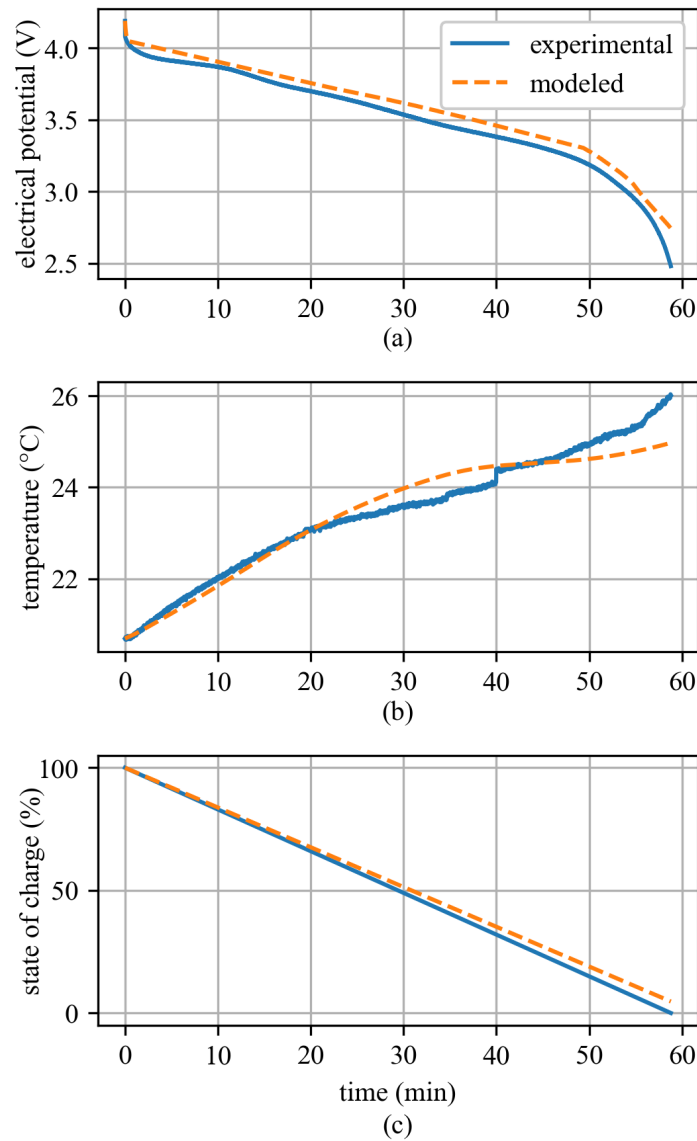


Figure 3.5 The a) voltage, b) temperature, and c) state of charge for a load profile as calculated by the model and tested experimentally.

imperfect tuning methods could lead to avoidable errors in prediction, therefore future work is required to optimize hyperparameters for deep neural networks. Second, noise in measurement requiring data windowing makes it difficult for the model to learn less significant relationships between variables, which could lead to over-generalization.

It should be noted that, while overestimating its contribution, the model appears to account for the entropic heating of the battery, evident by the accelerated temper-

ature increase at extremely low SOC. By training via an HPPC protocol, designed to highlight the more dynamic behavior, the neural networks successfully captured the nonlinear response exhibited by the battery. Furthermore, the model succeeds in both domains, also capturing nonlinearity in the electrical potential, observing both the initial and final voltage drops.

While able to operate with limited data, the DNNE is currently unaware to factors that cannot be seen from its input parameters. In the experimental data, SOC is calculated via coulomb counting using the current, and the neural network, acting as a linear regressor, calculates state of charge via the same method. However, it was assumed when determining the state of charge for the training data, that each cell had a perfect 3000 mAh capacity, when this is unlikely. Differences in the cell history or production could cause mismatches regarding the assumed nominal capacity, which the DNNE does not currently account for. In future model development, it is vital for accurate state of charge estimation that cells with documented history, or well measured initial capacity are used to account for differences in usable capacity.

3.5 CONCLUSION

This work presented a data-driven framework for modeling the electro-thermal response of lithium-ion batteries using a deep neural network ensemble (DNNE) trained on hybrid pulse power characterization (HPPC) data. The model predicted voltage, temperature, and state of charge under dynamic load conditions, achieving average absolute errors of 0.07 V, 0.25°C, and 2.35%, respectively. By deploying separate neural networks for each output domain and using windowed training data, the approach effectively captured nonlinear battery dynamics while reducing computational cost compared to physics-based models. This framework demonstrated a scalable and efficient alternative to traditional modeling techniques and established a foundation for future work in online learning and hybrid physics-informed architectures.

Future work will focus on implementing an online learning framework to enable continuous model adaptation as new operational data becomes available. Additional efforts will include refining the neural network architecture and expanding the training dataset to incorporate high C-rate discharge conditions, thereby improving model generalizability. Hybrid modeling approaches that integrate physics-based constraints with data-driven learning will also be explored to further enhance predictive accuracy. These developments aim to extend the applicability of deep learning in battery modeling and support more robust and scalable energy storage system optimization.

ACKNOWLEDGMENTS

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CHAPTER 4

PHYSICS-CONSTRAINED NEURAL NETWORKS FOR ELECTRO-THERMAL BATTERY MODELING AND EMULATION

This chapter is wholly based on “Physics-Constrained Neural Networks for Electro-Thermal Battery Modeling and Emulation,” accepted for presentation at the ASME IMECE 2026 Conference.

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4.1 ABSTRACT

The maritime industry is becoming increasingly dependent on battery energy storage for the ability to buffer and supply pulsed loads to optimize efficiency of onboard power system. When designing electrified shipboard power systems, battery test-

ing becomes expensive and time intensive, necessitating reliable models to emulate the electro-thermal response to loads. High fidelity physics-based methods can be computationally expensive and time consuming to parameterize. Thus, traditional physics-based models struggle with real-time digital twin applications, or hardware-in-the-loop testing. Alternatively, data driven methods have been explored, which are rapidly executable and less intensive to parameterize. However, they require obtaining large sets of expensive (time and cost) experimental data and struggle when loads or conditions differ from training data. To address limitations of both methods, this work proposes a physics constrained data-driven electro-thermal battery model that is more generalizable across a wider portion of the battery performance space than pure machine learning methods; while also requiring less data and being simpler to develop than traditional physics-based approaches. This is accomplished by constraining neural network during training using both an equivalent circuit model represent the electrical components and a differential equations for temperature. The network learns how the internal states, including open circuit voltage, RC relaxation pairs, and DC internal resistance, and entropic heat coefficient evolve with time and current. During training, the model is fit to the measured voltage and temperature, while penalized to obey the governing equations. Furthermore, the model parameters are bound to physically reasonable values. Across a dynamic load profile the model shows a 65.8 mV RMSE in electrical potential, and 0.205°C RMSE in temperature. Model generalization was tested with a constant current load greater than any within the training dataset, where the model exhibited a 49.0 mV RMSE in electrical potential, and 1.02 °C RMSE in temperature.

4.2 INTRODUCTION

Battery systems are playing an increasingly central role in more-electrified platforms, often used to smooth load fluctuations, increase efficiency, and meet pulsed load de-

mands in hybrid electric ships [17]. Across these applications, lithium-ion batteries are expected to operate not only as energy reservoirs, but also as dynamic components that interact continuously with power electronics, supervisory controllers, and thermal management systems [32]. As electrification expands into applications characterized by aggressive transients, pulse-power demands, and operation across broad environmental conditions, there is growing need for battery models that can reproduce both electrical and thermal behavior with sufficient fidelity for prediction, control development, safety analysis, and hardware or software validation [33]. In these settings, a model that captures terminal voltage alone is often insufficient. Voltage response, internal polarization, reversible and irreversible heat generation, and state evolution are tightly coupled, and modeling errors in one part of the system can propagate directly into erroneous predictions of power capability, thermal rise, or operational margin [34].

Equivalent-circuit models remain among the most widely used battery representations because they offer a practical compromise between physical interpretability and computational efficiency [35]. In contrast to high-fidelity electro-chemical models, equivalent-circuit models can often be evaluated rapidly enough for estimation, control, and hardware deployment applications while still preserving a structured relationship between internal states and terminal response [36]. However, conventional equivalent-circuit modeling workflows are often limited by the way parameters are identified and deployed. Often, parameter estimation is done through a sequence of independent fitting steps, lookup-table construction, manual interpolation, or hand-tuned parameter surfaces [37]. These procedures can become cumbersome when parameters vary strongly with state of charge and temperature, they may not generalize well when the battery is subjected to operating conditions outside the narrow subset used during identification. However, purely data-driven machine learning approaches have attracted increasing interest because of their ability to capture nonlinear rela-

tionships directly from experimental data [38]. Neural networks, in particular, can approximate highly nonlinear mappings between measured variables and battery response without requiring explicit derivation of every constitutive relationship [22]. Yet this flexibility comes with important drawbacks when applied without physical structure. A black-box model may fit training data well while producing nonphysical extrapolations, unrealistic internal trends, poor interpretability, or state evolutions that are difficult to reconcile with established battery behavior [39]. Model interpretability is a priority for many battery applications, especially those tied to estimation, control, and real-time deployment [40]. Quantities such as open-circuit voltage, ohmic resistance, entropic coefficient, and transient time scales carry direct physical meaning, and preserving that is vital for model trustworthiness and practical use.

Another challenge arises from parameter identifiability. Different experimental protocols excite different battery phenomena, and not all parameters are equally observable under all test conditions. Constant-current data may be well suited to reveal static voltage trends, baseline ohmic response, and thermal evolution over extended intervals, but it is not necessarily optimal for extracting fast and slow relaxation dynamics [41]. Conversely, pulse-power experiments such as hybrid pulse power characterization tests are specifically informative for transient polarization behavior and relaxation time scales, but are not the ideal source for establishing slower evolving or constant parameters of the model [42]. Attempting to learn all parameters simultaneously from all datasets can therefore blur the roles of individual parameters, reduce interpretability, and make optimization more sensitive to local minima or compensating errors between submodels.

These limitations motivate the need for a modeling framework that preserves the structure and interpretability of an electro-thermal equivalent-circuit representation while using machine learning only where it is most beneficial. To achieve this, a physics-constrained machine learning framework is developed to through neural ap-

proximators within a structured battery model. In this formulation, the neural networks serve as bounded maps for parameters that are expected to vary with state of charge and temperature, while the governing electrical and thermal equations remain explicitly defined. This approach allows the model to inherit the interpretability, deployability, and physical organization of a conventional equivalent-circuit model while benefiting from the expressiveness of machine learning, that could be implemented as outlined in figure 4.1.

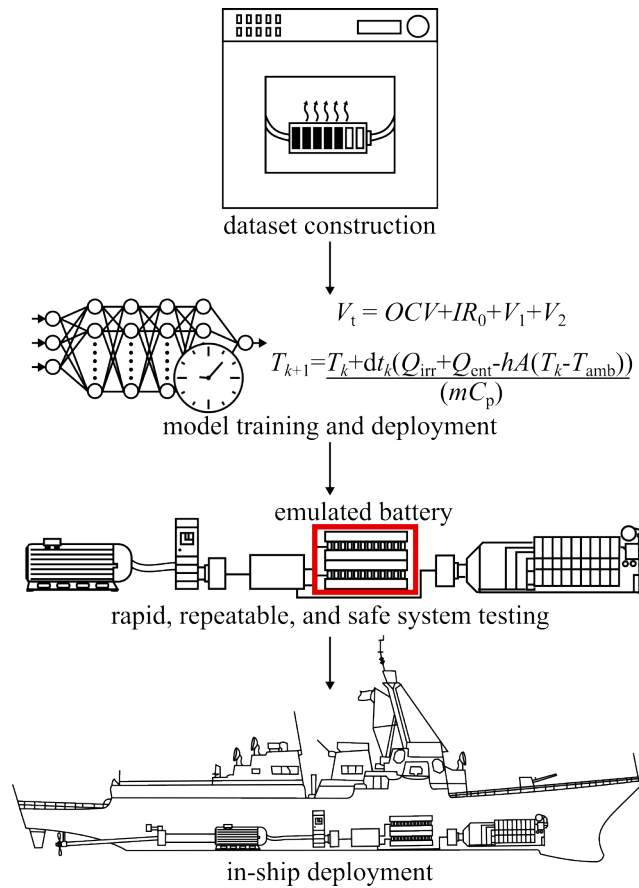


Figure 4.1 The process for developing and employing a battery emulator [1] through physics-constrained ML to improve system design and testing of advance shipboard architectures.

The resulting model combines learned nonlinear submodels for open-circuit voltage, ohmic resistance, and entropic behavior with a low-order dynamic RC structure for transient response. Physical bounds and regularization are incorporated to enforce

realistic behavior, and the electro-thermal formulation includes both irreversible and reversible heat generation. This produces a compact, interpretable model that can be deployed recursively under arbitrary current profiles while maintaining consistency between electrical and thermal predictions. The main contribution of this work is a physics-constrained machine learning framework for electro-thermal battery modeling that preserves the structure of an equivalent-circuit representation while learning non-linear state-dependent behavior directly from experimental data. The framework emphasizes interpretability, staged identification, and deployment-oriented performance, providing a practical pathway for integrating data-driven modeling into system-level battery applications.

4.3 METHODOLOGY

This work develops a two-stage physics-constrained electro-thermal equivalent-circuit model for lithium-ion batteries. The framework combines bounded neural network submodels for static and thermodynamic quantities with a 2nd-order dynamic RC representation for transient behavior. The objective is to produce a model that remains interpretable, computationally efficient, and suitable for recursive deployment, while still capturing nonlinear dependence of battery behavior on state of charge and temperature. To achieve this, the electrical and thermal backbone is first identified from constant-current data, after which the dynamic polarization parameters are identified from Pulse Power Characterization (HPPC) data while the previously learned submodels are held fixed.

The public dataset used in this work [43] was previously used in a pure data driven modeling approach and is discussed in detail by Madden et al. [16]. This dataset consist of testing a single 3.6V 3000 mAh lithium nickel manganese cobalt (NMC) 18650 cell (Samsung 30Q) under constant current and HPPC tests. The cell was tested using a battery cycling system (NHR-9200) while held in a environmental

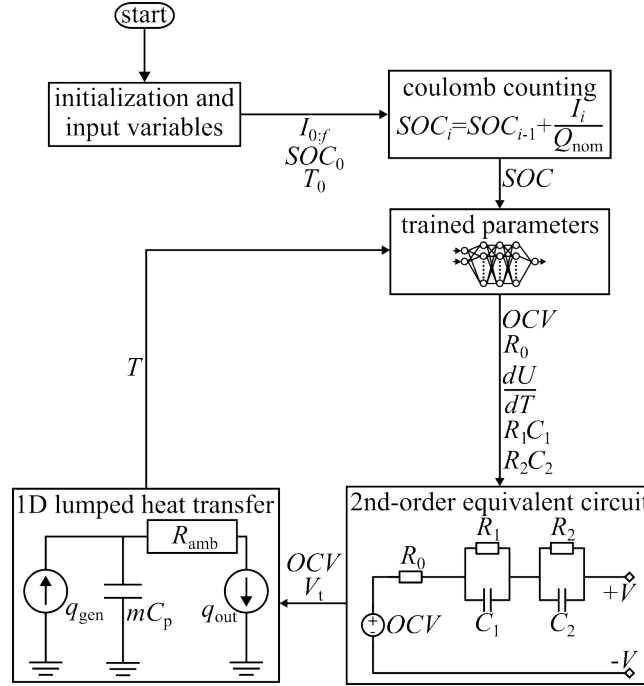


Figure 4.2 A diagram of the information exchanged between submodels of the electro-thermal physics-constrained ML model.

chamber (IncuFridge Pro 328) to maintain a constant temperature. All sampling was done at 1 S/s.

4.3.1 ELECTRO-THERMAL MODEL STRUCTURE AND PARAMETERIZATION

Shown in figure 4.2, the deployed model is formulated as an electro-thermal equivalent-circuit representation driven by an input current profile. At each time-step, the model receives the current I_k , time-step duration Δt_k , ambient temperature $T_{amb,k}$, and the current internal state. The internal state consists of the state of charge SOC_k , cell temperature T_k , and two RC polarization states, $v_{1,k}$ and $v_{2,k}$. The model then evaluates a set of learned and identified submodels to update voltage, thermal behavior, and state evolution.

The terminal voltage is expressed as

$$V_k = OCV(SOC_k, T_k) + I_k R_0(SOC_k, T_k) + v_{1,k} + v_{2,k}, \quad (4.1)$$

where $OCV(SOC, T)$ is the open-circuit voltage surface, $R_0(SOC, T)$ is the ohmic

resistance surface, and v_1, v_2 are polarization-state voltages associated with a second-order RC representation. The sign convention in (4.1) follows the implementation used throughout the framework and is retained consistently in training and deployment.

The polarization states evolve according to

$$a_1 = \exp\left(-\frac{\Delta t_k}{R_1 C_1}\right), \quad a_2 = \exp\left(-\frac{\Delta t_k}{R_2 C_2}\right), \quad (4.2)$$

$$v_{1,k+1} = a_1 v_{1,k} + (1 - a_1) I_k R_1, \quad (4.3)$$

$$v_{2,k+1} = a_2 v_{2,k} + (1 - a_2) I_k R_2. \quad (4.4)$$

Here, R_1, C_1, R_2 , and C_2 are treated as static parameters that are identified from pulse-power data and then used as fixed global values during deployment. In this form, R_1 and R_2 govern the magnitudes of the polarization responses, while $R_1 C_1$ and $R_2 C_2$ determine the associated relaxation time scales.

The state of charge is advanced through coulomb counting,

$$SOC_{k+1} = SOC_k + \frac{I_k \Delta t_k}{Q_{\text{nom}}}, \quad (4.5)$$

where Q_{nom} is the rated cell capacity in coulombs. During recursive rollout, the state of charge is clipped to the range $[0, 1]$ to prevent drift outside the domain spanned by the training data. This ensures that the learned submodels are evaluated only within a physically meaningful range.

The thermal model is formulated as a lumped energy balance with irreversible and reversible heat generation,

$$q_{\text{irr},k} = |I_k| |OCV(SOC_k, T_k) - V_k|, \quad (4.6)$$

$$q_{\text{ent},k} = I_k T_k \frac{dU}{dT}(SOC_k), \quad (4.7)$$

$$T_{k+1} = T_k + \Delta t_k \frac{q_{\text{irr},k} + q_{\text{ent},k} - hA(T_k - T_{\text{amb}})}{mC_p}, \quad (4.8)$$

where mC_p is the effective thermal capacitance and hA is the lumped convective heat transfer coefficient. The term $dU/dT(SOC)$ is a learned entropic coefficient that captures the reversible thermal contribution as a function of state of charge.

Equations (4.1)–(4.8) define the complete deployed model. Given an initial condition $(SOC_0, T_0, v_{1,0}, v_{2,0})$ and an input current profile, the model may be iterated forward to predict terminal voltage, state of charge, cell temperature, and internal polarization-state evolution.

The deployed model depends on three learned submodels and four identified static parameters.

First, the open-circuit voltage submodel $OCV(SOC, T)$ is represented by a bounded neural network taking state of charge and normalized temperature as inputs. The architecture emphasizes state of charge as the dominant variable while allowing a smaller learned temperature correction. This choice reflects the expectation that OCV depends primarily on state of charge, with temperature introducing a secondary shift.

Second, the ohmic resistance submodel $R_0(SOC, T)$ is represented by a bounded neural network with the same inputs. As with the OCV model, the parameterization is structured so that SOC contributes the dominant effect, while temperature acts as a weaker correction. This allows the model to capture practical dependence of ohmic response on both electro-chemical state and thermal state.

Third, the entropic coefficient $dU/dT(SOC)$ is represented by a bounded neural network depending only on state of charge. Restricting this quantity to an SOC-only function reduces entanglement with the explicit temperature dependence already present in $OCV(SOC, T)$ and $R_0(SOC, T)$, while preserving a physically interpretable reversible heat term.

Each neural submodel uses a bounded output transform of the form

$$\hat{y} = y_{\min} + (y_{\max} - y_{\min}) \sigma(z), \quad (4.9)$$

where z is the raw network output and $\sigma(\cdot)$ is the logistic sigmoid. This guarantees that each learned quantity remains within a prescribed physical range throughout training and deployment.

The dynamic polarization parameters R_1 , C_1 , R_2 , and C_2 are not represented by neural networks. Instead, they are treated as static positive parameters identified from HPPC data. Positivity is enforced during optimization by learning unconstrained variables that are mapped through a softplus transform. Therefore, the resulting deployment model consists of nonlinear learned surfaces for static and thermodynamic behavior, combined with a conventional second-order RC transient structure for dynamic polarization behavior.

4.3.2 TRAINING PROCEDURE

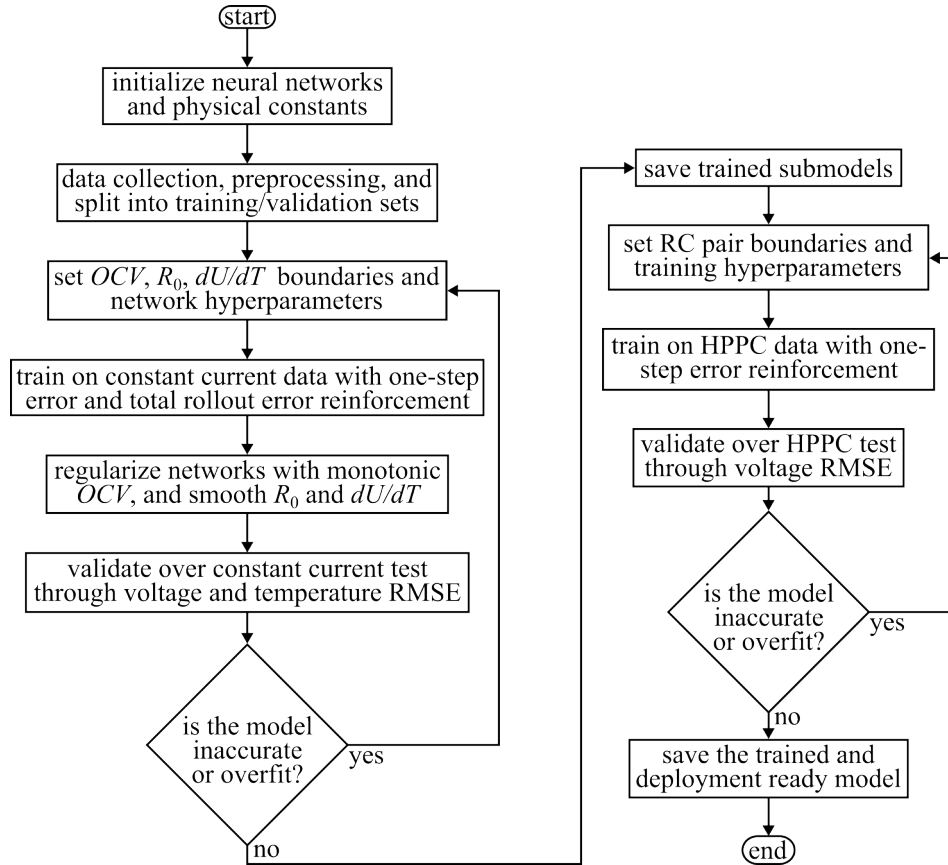


Figure 4.3 A flowchart explaining the training process of the electro-thermal physics-constrained ML battery model.

Outlined in figure 4.3, the training process is divided into two stages so that different experimental datasets inform different portions of the deployed model. Constant-current data is used to learn the static and thermodynamic submodels, while HPPC data is used to identify the dynamic polarization parameters. This is done because long constant-current experiments provide strong information for OCV behavior, ohmic response, and temperature evolution, whereas pulse-power experiments provide much stronger excitation of the dynamic RC states. Furthermore, this prevents the networks from attributing pulse behavior to false OCV drops or ohmic spikes, which is more likely when data is limited.

All datasets contain the columns current, voltage, temperature, and soc. If a time column is present, the time-step sequence is inferred directly from it; otherwise a unit time-step is assumed. For each file, the current history, measured voltage, temperature, state of charge, and ambient temperature history are assembled into a sequence record.

Because experimental files can have different durations, all files in a stage are padded to the maximum sequence length in the batch. A binary mask $m_{k,b} \in \{0, 1\}$ is constructed to indicate whether time-step k of file b corresponds to a valid sample or a padded entry. This mask is applied to every data-fit loss, ensuring that padded values do not influence optimization. For a generic error sequence $e_{k,b}$, the masked mean for file b is computed as

$$\mathcal{L}_b = \frac{\sum_k m_{k,b} e_{k,b}}{\sum_k m_{k,b} + \varepsilon}, \quad (4.10)$$

where ε is a small positive constant for numerical stability. Stage losses are then formed by averaging these per-file quantities across files, so that long records do not dominate the optimization solely because they contain more time-steps, often due to lower currents.

For stage 1, the constant-current dataset is additionally split into a training subset and a held-out validation subset. The validation set is used only for total profile

evaluation and model selection.

Stage 1 is designed to identify the electro-thermal backbone of the deployed model. The three trainable submodels in this stage are $OCV(SOC, T)$, $R_0(SOC, T)$, and $dU/dT(SOC)$. To improve both training stability and performance, stage 1 uses a hybrid objective consisting of teacher-forced, or one-step, losses and free-rollout, or total profile, losses.

In the teacher-forced branch, the measured state trajectories are used as inputs to the learned submodels. Specifically, the networks are evaluated on the measured state of charge and measured temperature histories,

$$\widehat{OCV}_{k,b} = OCV(SOC_{k,b}^{\text{meas}}, T_{k,b}^{\text{meas}}), \quad (4.11)$$

$$\hat{R}_{0,k,b} = R_0(SOC_{k,b}^{\text{meas}}, T_{k,b}^{\text{meas}}), \quad (4.12)$$

$$\frac{\widehat{dU}}{dT}_{k,b} = \frac{dU}{dT}(SOC_{k,b}^{\text{meas}}). \quad (4.13)$$

These are used to compute a teacher-forced voltage prediction,

$$V_{k,b}^{\text{teacher}} = \widehat{OCV}_{k,b} + I_{k,b} \hat{R}_{0,k,b}, \quad (4.14)$$

and a one-step teacher-forced temperature prediction,

$$T_{k+1,b}^{\text{teacher}} = T_{k,b}^{\text{meas}} + \Delta t_{k,b} \cdot \frac{q_{\text{irr},k,b}^{\text{teacher}} + q_{\text{ent},k,b}^{\text{teacher}} - hA(T_{k,b}^{\text{meas}} - T_{\text{amb},k,b})}{mC_p}, \quad (4.15)$$

where the heat terms are evaluated using the teacher-forced states. This branch encourages accurate local behavior when the state trajectory is known.

However, one-step accuracy alone does not guarantee good recursive performance. To address this, stage 1 also includes a free-rollout branch. For each sequence, the simulation is initialized from the first measured state,

$$SOC_{0,b} = SOC_{0,b}^{\text{meas}}, \quad T_{0,b} = T_{0,b}^{\text{meas}}, \quad (4.16)$$

and is then advanced according to (4.1)–(4.8) with $v_1 = v_2 = 0$. In other words, the model uses its own predicted SOC_k and T_k to evaluate OCV , R_0 , and dU/dT

at every subsequent time-step. This branch exposes the model to the same recursive error accumulation that arises during deployment.

The voltage and temperature data-fit terms are therefore constructed as

$$\mathcal{L}_{V,\text{teacher}} = \frac{1}{B} \sum_{b=1}^B \frac{\sum_k m_{k,b} (V_{k,b}^{\text{teacher}} - V_{k,b}^{\text{meas}})^2}{\sum_k m_{k,b} + \varepsilon}, \quad (4.17)$$

$$\mathcal{L}_{T,\text{teacher}} = \frac{1}{B} \sum_{b=1}^B \frac{\sum_k m_{k,b} (T_{k,b}^{\text{teacher}} - T_{k,b}^{\text{meas}})^2}{\sum_k m_{k,b} + \varepsilon}, \quad (4.18)$$

$$\mathcal{L}_{V,\text{free}} = \frac{1}{B} \sum_{b=1}^B \frac{\sum_k m_{k,b} (V_{k,b}^{\text{free}} - V_{k,b}^{\text{meas}})^2}{\sum_k m_{k,b} + \varepsilon}, \quad (4.19)$$

$$\mathcal{L}_{T,\text{free}} = \frac{1}{B} \sum_{b=1}^B \frac{\sum_k m_{k,b} (T_{k,b}^{\text{free}} - T_{k,b}^{\text{meas}})^2}{\sum_k m_{k,b} + \varepsilon}. \quad (4.20)$$

To encourage physically plausible submodels, several regularization terms are added. First, a monotonicity penalty is imposed on negative values of $\partial OCV / \partial SOC$,

$$\mathcal{L}_{\text{mono}} = \frac{\sum_i \max(0, -\frac{\partial OCV_i}{\partial SOC_i})}{N + \varepsilon}, \quad (4.21)$$

where the derivatives are obtained by automatic differentiation over the flattened training batch. Second, a smoothness penalty is applied to the resistance surface,

$$\mathcal{L}_{R_0,\text{smooth}} = \frac{\sum_i \left[\left(\frac{\partial R_{0,i}}{\partial SOC_i} \right)^2 + 0.1 \left(\frac{\partial R_{0,i}}{\partial T_i} \right)^2 \right]}{N + \varepsilon}, \quad (4.22)$$

and a smoothness penalty is also applied to the entropic coefficient,

$$\mathcal{L}_{dU/dT,\text{smooth}} = \frac{\sum_i \left(\frac{\partial (dU/dT)_i}{\partial SOC_i} \right)^2}{N + \varepsilon}. \quad (4.23)$$

Finally, a variance-floor penalty discourages collapse of the OCV surface toward a constant output,

$$\mathcal{L}_{OCV,\text{var}} = \max(0, \delta - \text{Var}(OCV)), \quad (4.24)$$

where δ is a small target variance threshold.

The full stage-1 loss is then written as

$$\begin{aligned} \mathcal{L}_{\text{stage1}} = & w_{V,\text{teacher}}\mathcal{L}_{V,\text{teacher}} + w_{T,\text{teacher}}\mathcal{L}_{T,\text{teacher}} + w_{V,\text{free}}\mathcal{L}_{V,\text{free}} + w_{T,\text{free}}\mathcal{L}_{T,\text{free}} \\ & + \lambda_{\text{mono}}\mathcal{L}_{\text{mono}} + \lambda_{R_0}\mathcal{L}_{R_0,\text{smooth}} + \lambda_{OCV}\mathcal{L}_{OCV,\text{var}} + \lambda_{dU/dT}\mathcal{L}_{dU/dT,\text{smooth}}. \end{aligned} \quad (4.25)$$

Stage 1 training is performed in two phases. During the warmup phase, the teacher-forced terms retain substantial weight to stabilize the learned constitutive surfaces. During the fine-tuning phase, the free-rollout terms are emphasized more strongly so that the model is optimized toward longer term deployment performance. The stage-1 parameters are selected using the held-out constant-current validation set, where total iteration voltage RMSE and temperature RMSE are computed periodically. The best stage-1 weights are retained according to this validation criterion.

Once stage 1 is complete, the learned submodels $OCV(SOC, T)$, $R_0(SOC, T)$, and $dU/dT(SOC)$ are no longer trainable. Stage 2 then uses HPPC data to identify the dynamic polarization parameters R_1 , C_1 , R_2 , and C_2 .

During stage 2, the frozen submodels are evaluated using the measured SOC and temperature histories from the HPPC data, yielding the quasi-static voltage and thermal quantities required by the full deployed model. The dynamic RC states are then rolled out according to (4.2)–(4.4) using candidate values of R_1 , C_1 , R_2 , and C_2 . The resulting terminal voltage and one-step thermal predictions are compared against the measured HPPC trajectories.

The stage-2 voltage and thermal losses are defined in the same per-file masked form as in stage 1, and a weak prior is also applied to discourage excessive departure from the initial RC guesses,

$$\mathcal{L}_{RC,\text{prior}} = \frac{(R_1 - R_{1,0})^2}{R_{1,0}^2 + \varepsilon} + \frac{(C_1 - C_{1,0})^2}{C_{1,0}^2 + \varepsilon} + \frac{(R_2 - R_{2,0})^2}{R_{2,0}^2 + \varepsilon} + \frac{(C_2 - C_{2,0})^2}{C_{2,0}^2 + \varepsilon}, \quad (4.26)$$

where $R_{1,0}$, $C_{1,0}$, $R_{2,0}$, and $C_{2,0}$ are the chosen initial guesses.

The full stage-2 loss is therefore

$$\mathcal{L}_{\text{stage2}} = w_{V,\text{stage2}}\mathcal{L}_{V,\text{stage2}} + w_{T,\text{stage2}}\mathcal{L}_{T,\text{stage2}} + \lambda_{RC}\mathcal{L}_{RC,\text{prior}}. \quad (4.27)$$

Only the four scalar RC parameters are trainable in stage 2. They are optimized using Adam, and early stopping is used to terminate the procedure once the stage-2 loss ceases to improve. The best identified parameter values are then saved together with the frozen stage-1 submodels to form the final deployable electro-thermal model.

4.4 RESULTS

To understand model reliability, the physics constrained networks were tested across three load types. First, the model is evaluated on a 4C constant current test, to assess the fit of the more impactful learned parameters including OCV , R_0 , and dU/dT , as well as model generalizability, as only rates below 3C were used in training. The RC-pairs, R_1C_1 and R_2C_2 are assessed under an HPPC profile to display model performance under dynamic load.

Displayed in figure 4.4, model performance across a 4C, or 12 A, constant current discharge is shown. It can be seen that the model shows good agreement above 20% SOC, despite training on a maximum rate of 9 A. A significant source of error could stem from the profile extending beyond the temperature bounds of the training data, due to the discharge rate also exceeding the data trained on. The cell surpasses 55°C, the high temperature trained on, at ~12 min. This would align with 80% depth of discharge during a 4C constant current test, which is when the modeled voltage deviates from the experimental data. Despite the observed error at low SOC, 49.0 mV RMSE in electrical potential, and 1.02 °C RMSE in temperature is acceptable as battery behavior becomes significantly more difficult to model at high C-rates (>2C) [44].

The model shows good electrical agreement over an HPPC profile seen in figure 4.5, containing a discharge and charge pulse at every 5% SOC, showcasing the dynamic capability of the model. During training, the model saw limited exposure to HPPC data, only 3 profiles, due to long training times, highlighting one limitation

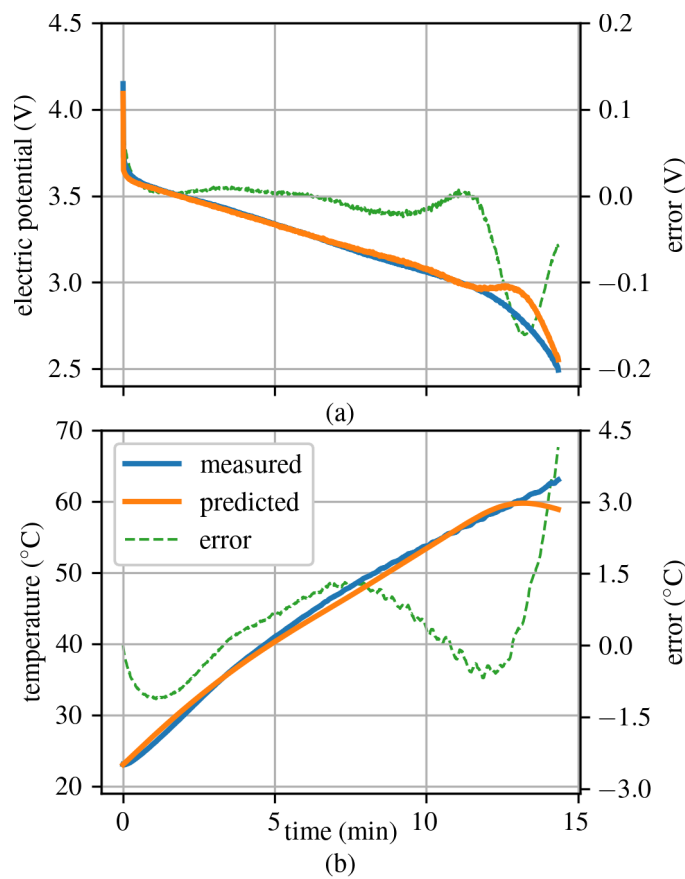


Figure 4.4 The modeled and experimental (a) voltage and (b) temperature across a 4C (12 A) constant current discharge at room temperature ($\sim 23^{\circ}\text{C}$ ambient).

of the proposed training framework. However, the model shows a 65.8 mV RMSE in electrical potential, and 0.205°C RMSE in temperature, across a 1C HPPC profile at 30°C . It was assumed that all experimental data remained within the SOC range $[0, 1]$. This could be a significant source of error, as experimental voltage drops below 2.5 V, signifying an over discharge on the final pulse. Disparity between modeled and experimental SOC could contribute to the error in voltage noticeable below $\sim 15\%$ SOC. Furthermore, an over discharge would likely contribute to considerable heat generation during the final discharge, where the temperature error is the greatest.

A primary limitation of the proposed methodology lies in the separation of parameter identification across datasets and model components. While the staged approach improves observability, it implicitly assumes that these behaviors are decoupled and

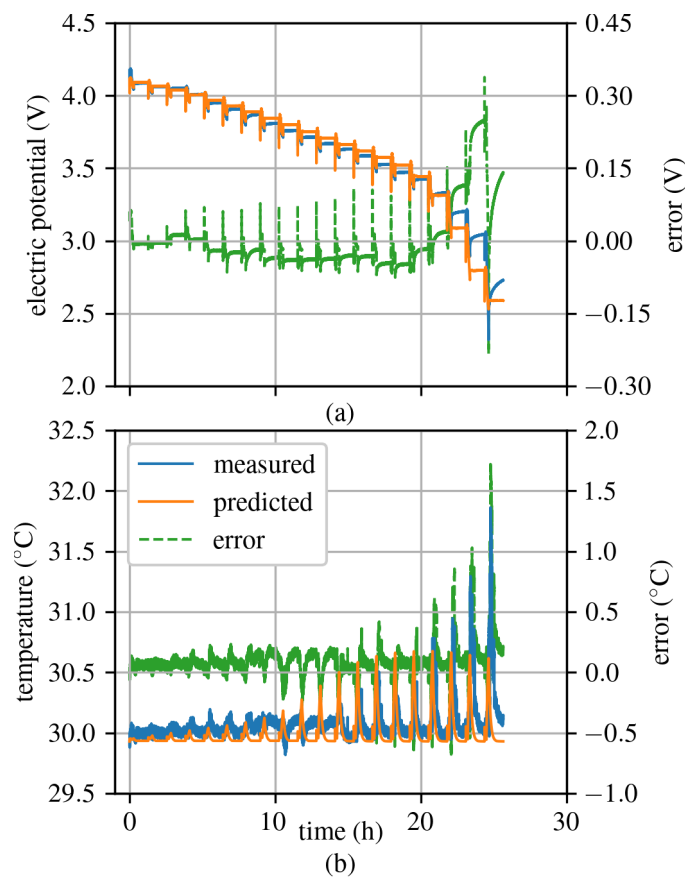


Figure 4.5 The modeled and experimental (a) voltage and (b) temperature across an HPPC profile in a 30°C ambient temperature chamber, containing 1C (3 A) pulses every 5% SOC, and C/3 (1 A) discharges between each pulse.

transferable across operating conditions. In practice, parameters such as polarization dynamics and thermal response can exhibit dependence on SOC, temperature, and even aging state. By enforcing static R_1 , C_1 , R_2 , C_2 values and learning OCV , R_0 , and dU/dT independently, the model may compensate for unmodeled coupling through the learned submodels, potentially leading to parameter bias or reduced generalization outside the training domain. Additionally, the reliance on bounded neural networks constrains outputs to physically reasonable ranges but may also limit the model's ability to capture edge-case behavior near operational limits, particularly under extreme currents or temperatures not well represented in the training data.

Another important source of error arises from the deployment structure and the underlying modeling assumptions. The lumped thermal model assumes spatially uni-

form temperature and simplified heat transfer via a constant hA , which neglects internal gradients and dynamic cooling effects present in real systems. Similarly, the use of coulomb counting for SOC propagation introduces cumulative error sensitivity, particularly if the initial SOC is uncertain or if current measurements contain bias. During training, the combination of one-step and total iteration losses mitigates but does not eliminate error accumulation, meaning small discrepancies in learned relationships can compound over long horizons. Finally, measurement noise, sensor calibration errors (especially in temperature), and inconsistencies between datasets (e.g., differing ambient conditions or instrumentation) can introduce discrepancies that the model may inadvertently learn as physical behavior, reducing predictive fidelity during deployment on unseen data.

4.5 CONCLUSION

This work presented physics-constrained ML for electro-thermal modeling of lithium-ion batteries. By embedding an equivalent-circuit representation and governing thermal equations directly into the neural network training process, the proposed framework preserves physical interpretability and computational efficiency while improving generalization beyond the training domain. Across a dynamic load profile the model shows a 65.8 mV RMSE in electrical potential, and 0.205°C °C RMSE in temperature. Model generalization was tested with a constant current load greater than any within the training dataset, where the model exhibited a 49.0 mV RMSE in electrical potential, and 1.02 °C RMSE in temperature. The two-stage identification strategy further enables robust separation of static, dynamic, and thermodynamic effects, making the model suitable for real-time applications such as digital twins and hardware-in-the-loop testing.

Future work includes model adaptation to new data as collected while under deployment through the development of an online learning framework. Additionally,

effort will be made to minimize model training time and computation resources. Thus, encouraging tuning optimization to enable high fidelity performance.

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CHAPTER 5

CONCLUSION

5.1 CONCLUSION

This work investigated a series of electro-thermal battery modeling approaches aimed at supporting real-time battery emulation. The first approach highlighted a physics-based electro thermal hardware-in-the-loop battery emulator that demonstrated the feasibility of reproducing voltage and temperature behavior in real-time. Building on this foundation, a deep neural network framework was developed to learn electro thermal battery behavior directly from experimental data. Finally, a physics informed machine learning framework was explored to combine the interpretability and structure of physics based models with the adaptability of machine learning. Together, these studies demonstrate the strengths and limitations of physics based, data driven, and physics informed approaches while highlighting the potential of physics informed machine learning as a pathway toward more accurate and deployable battery models.

5.2 CHALLENGES

Despite the promising results presented in this thesis, several challenges remain. Battery characterization requires extensive testing across temperatures, operating conditions, and states of charge, while thermal measurements are often noisy and subject to experimental uncertainty. Physics based models require parameter identification and rely on simplifying assumptions that may limit fidelity. Data driven models remain dependent on the quality and diversity of training data and can struggle to generalize

beyond observed operating conditions. Recursive prediction approaches may accumulate error over long horizons, and purely data driven models may violate known physical behavior. Although physics informed machine learning addresses many of these shortcomings, selecting appropriate physical constraints remains challenging, as excessive constraints may reduce flexibility while insufficient constraints may fail to provide meaningful physical guidance. Additional challenges remain regarding real time implementation, pack level scaling, integration with battery management systems, and validation under highly dynamic operating conditions.

5.3 FUTURE DIRECTION

Future directions should pursue expanding the physics informed machine learning framework through both improved physical representations and adaptive learning capabilities. The models developed in this thesis primarily employ constraints derived from equivalent circuit models due to their computational efficiency and suitability for real time applications. However, future work could investigate incorporating additional electrochemical information derived from higher fidelity models such as the Single Particle Model, Single Particle Model with Electrolyte, or the Doyle Fuller Newman pseudo two dimensional model. Constraints related to lithium diffusion, reaction kinetics, electrolyte transport, and concentration dynamics may improve model fidelity while preserving the flexibility of machine learning.

Another promising direction is the adoption of online learning frameworks that allow models to adapt as new battery data becomes available during operation. Because battery characteristics evolve with aging, degradation, and environmental conditions, a model trained once may gradually lose accuracy over time. Online learning would allow the model to continuously update itself using incoming measurements of voltage, current, temperature, and other battery states. When combined with physics informed constraints, such an approach could maintain accuracy throughout the bat-

tery lifetime while preserving physical consistency and reducing the need for repeated characterization testing.

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APPENDIX A

REPRINT PERMISSIONS

A.1 CHAPTER 1: ELECTRO-THERMAL HARDWARE-IN-THE-LOOP BATTERY EMULATOR FOR SHIPBOARD SYSTEMS TESTING

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