

Data-Driven PHM with BDPS Tool Suite: Battery Data Acquisition for Degradation Modeling

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Abstract— The Battery Diagnostics and Prognostics System (BDPS) Tool Suite advances Prognostics and Health Management (PHM) through its innovative Data Acquisition (DA) Toolbox, the backbone for robust data collection, degradation modeling, and lifecycle prediction. Operating at 1 Hz with 0.05% voltage accuracy and ± 5 mA current precision, the DA Toolbox integrates with battery cyclers to collect real-time voltage, current, capacity, and temperature data across -30°C to 60°C and varying C-rates for NMC, LFP, and NCA chemistries. This data drives hybrid models blending empirical trends with electrochemical simulations to reveal degradation mechanisms like capacity fade, temperature spikes, SEI growth, lithium plating, loss of active material (LAM), and loss of lithium inventory (LLI). Using the Adaptive Remaining Useful Life Estimator (ARULE), BDPS delivers 95% accurate SoH and RUL predictions over 500+ lithium-ion cycles. The DA Toolbox’s affordability, modularity, and secure CSV/JSON data management with cloud synchronization enhance accessibility and scalability for startups, labs, and industry, providing actionable insights for maintenance and resilience in applications like electric vehicles (EVs) and grid-energy storage.

Keywords— Battery Diagnostics, Prognostics and Health Management (PHM), Data Acquisition (DA), Sensors, Battery Degradation, Modeling, Lithium-Ion Batteries, Hybrid Modeling

I. INTRODUCTION

The rapid integration of lithium-ion (Li-ion) batteries into electric vehicles (EVs), grid-scale energy storage, and portable electronics has increased the demand for Prognostics and Health Management (PHM) systems to monitor and predict degradation profiles. Data-driven PHM leverages high-fidelity cycling data to model complex degradation phenomena, including capacity fade from solid electrolyte interphase (SEI) growth, lithium plating-induced short circuits, and impedance rise from active material pulverization. Commercial battery cyclers, however, impose a steep financial barrier, often exceeding \$1000/channel, making them inaccessible to small-scale researchers, startups, and emerging industries. This paper introduces the data acquisition (DA) toolbox framework, a low-cost (less than \$100/channel) cycling test system engineered with modular hardware and advanced data acquisition capabilities. This toolbox is integrated within the Battery Diagnostic and Prognostic System (BDPS) Tool Suite comprising degradation modeling algorithms along with IEEE 1856-2017 [1] architecture to enable scalable, industry-relevant PHM.

Early detection of degradation is crucial for optimizing battery lifespan, safety, and economic viability. SEI formation initiates within the first 10–20 cycles as electrolyte decomposes at the anode, consuming up to 10% of initial capacity, while lithium plating—triggered by high C-rates ($>1\text{C}$) or low temperatures ($<0^{\circ}\text{C}$)—emerges within 50 cycles, reducing cycleable lithium and risking dendrite growth [2]. These early processes, if unaddressed, accelerate subsequent degradation, such as cathode electrolyte interphase (CEI) formation and particle cracking, with capacity fade rates escalating from 0.1% to 0.5% per cycle under abusive conditions (e.g., 2C charging at 45°C) [3]. Early PHM intervention—such as optimizing charge-discharge protocols or enhancing thermal management—can mitigate these effects, reducing safety hazards and extending service life [2]. Affordable testing platforms are thus essential to capture these initial signatures across diverse operating conditions.

Recent advancements in low-cost battery cycling systems underscore their transformative potential to address the growing demand for accessible Prognostics and Health Management (PHM) in lithium-ion battery applications. Von Bülow et al. developed a fleet-scale tester leveraging Raspberry Pi controllers, achieving a remarkable 95% State of Health (SoH) prediction accuracy for EV batteries under dynamic discharge profiles (0.5C–2C), with a current precision of ± 1 mA across 1–5 A ranges [4]. This system slashes costs by 80% compared to commercial testers like Maccor or BioLogic, which often exceed \$10,000 per channel, making it viable for large-scale fleet monitoring [1]. Attia et al. pioneered a machine learning-driven approach using low-cost setups—such as basic potentiostats and open-source hardware—to predict cycle life with an $R^2 > 0.9$ across hundreds of cycles, reducing testing time from over 500 days to 16 days by optimizing fast-charging protocols (e.g., 4C to 80% SoC) [5]. Their work leverages datasets from simple setups to model degradation under realistic conditions, including temperature variations and partial SoC cycling. Che et al. review a range of affordable systems capturing aging data across -20°C to 45°C , achieving SoH estimation errors below 2% through techniques like incremental capacity analysis (ICA) and differential voltage analysis (DVA), even with low-cost sensors sampling at 1 Hz [2]. These innovations tackle a critical limitation: conventional PHM studies predominantly rely on high-end cyclers that fail to replicate real-world stressors—such as partial SoC cycling (20–80%), fast-charging regimes (up to 3C), and thermal gradients—thus limiting model

generalizability, as noted by Kumar and Das [6]. The DA Toolbox in the BDPS Tool Suite builds on this momentum, offering high-resolution logging (1 Hz sampling rate, 0.05% voltage precision across 2.5–4.2 V) and advanced algorithms to track capacity fade (e.g., from 100% to 80% over 500 cycles). By integrating cost-effective hardware with sophisticated data processing, BDPS democratizes PHM, enabling researchers and industries to study degradation under diverse, realistic scenarios.

The stakes of early degradation management extend far beyond mere performance metrics, encompassing critical safety risks, economic burdens, and operational sustainability, particularly as EV adoption accelerates globally. Kumar and Das report that undetected lithium plating—often triggered by high-rate charging (e.g., 2C) or low temperatures ($<0^{\circ}\text{C}$)—doubles thermal runaway likelihood after 200 cycles, with internal short circuits increasing failure rates by up to 15% in NMC cells under abusive conditions [6]. Das Goswami et al. Reported that undetected battery degradation could escalate into thermal runaway, posing significant safety risks as shown in Figure 1. [7-9]



Figure 1. Examples of lithium-ion battery-related fire incidents, highlighting the risks of thermal runaway in consumer electronics and electric vehicles. (Top) A laptop fire (Source: BBC); (Middle) Multiple vehicles engulfed in flames (Source: BBC); (Bottom) An electric vehicle fire on a roadway (Source: ABC News).

Birkel et al. further detail how plating, detectable via voltage plateaus and capacity drops within 50–100 cycles, compromises cell integrity, raising the risk of catastrophic events like fires, a concern amplified by the 750 GWh of EV battery demand in 2023 [3]. Economically, early capacity fade, typically 5–10% within the first 20 cycles due to SEI growth, can be linked to

downstream warranty costs, projecting a \$1–2 billion annual burden for OEMs as EV fleets expand, compounded by reduced range and premature pack replacement. The BDPS's affordability and adaptability enable proactive monitoring, leveraging its high-fidelity data acquisition to flag plating and fade early, thus reducing risks of catastrophic failure and supporting cost-sensitive applications like fleet management and second-life storage, where cells retain 70–80% capacity post-EV use. This paper elaborates the BDPS's DA Toolbox's and application, establishing it as a pivotal tool for industry-driven battery health management (HM) by bridging the gap between cost, safety, and innovation.

II. SYSTEM ARCHITECTURE

The Battery Diagnostic and Prognostic System (BDPS) Tool Suite provides a comprehensive and modular framework engineered specifically for scalable, affordable, and precise battery prognostics and health management (PHM). The BDPS architecture integrates five central subsystems: the Data Acquisition (DA) Toolbox, Modeling Toolbox, and Analysis Toolbox, Advisory Generation (AG) Toolbox, and Health Management (HM) Toolbox which are all designed in alignment with the IEEE 1856-2017 PHM standard [1]. At the foundation of this integrated architecture is the DAQ Toolbox, strategically developed to bridge the critical gap between high-end battery cyclers and cost-effective testing setups suitable for small-scale research groups, startups, and emerging battery technology companies.

The DAQ Toolbox comprises low-cost and low size, weight, and power (SWaP) modular hardware interfaces, designed for seamless compatibility with widely-used cycling hardware such as the commercial-off-the-shelf (COTS) ZKETECH EBC-A10H and EBC-A20H battery cyclers. The cycler communicates with the test computer/system through a serial interface, while affordable COTS microcontrollers like Seeed Studio ESP32C or XIAO-NRF52840 interfaced with the Adafruit MAX31855 Thermocouple Breakout are used to measure battery temperature through serial, Wi-Fi, or Bluetooth Low Energy (BLE) interfaces. Shown in Figure 2 is how each battery test system comprising the cycler and microcontroller is interfaced with the testing computer hosting the BDPS Tool Suite with the DAQ Toolbox.

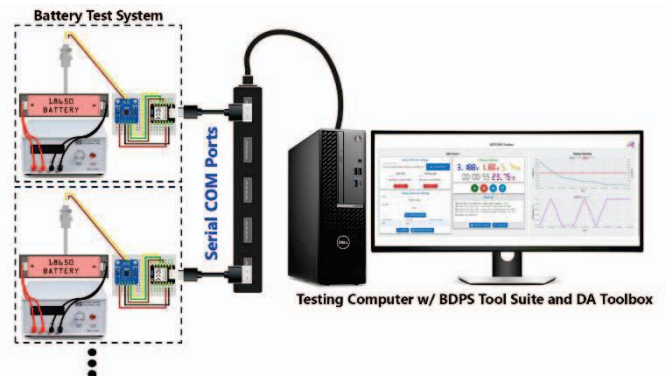


Figure 2. The BDPS Data Acquisition (DA) Architecture wherein a single or multiple Battery Test System(s) can be connected to a testing computer via COM ports and a serial interface, utilizing the BDPS Tool Suite and DA Toolbox for battery degradation DA.

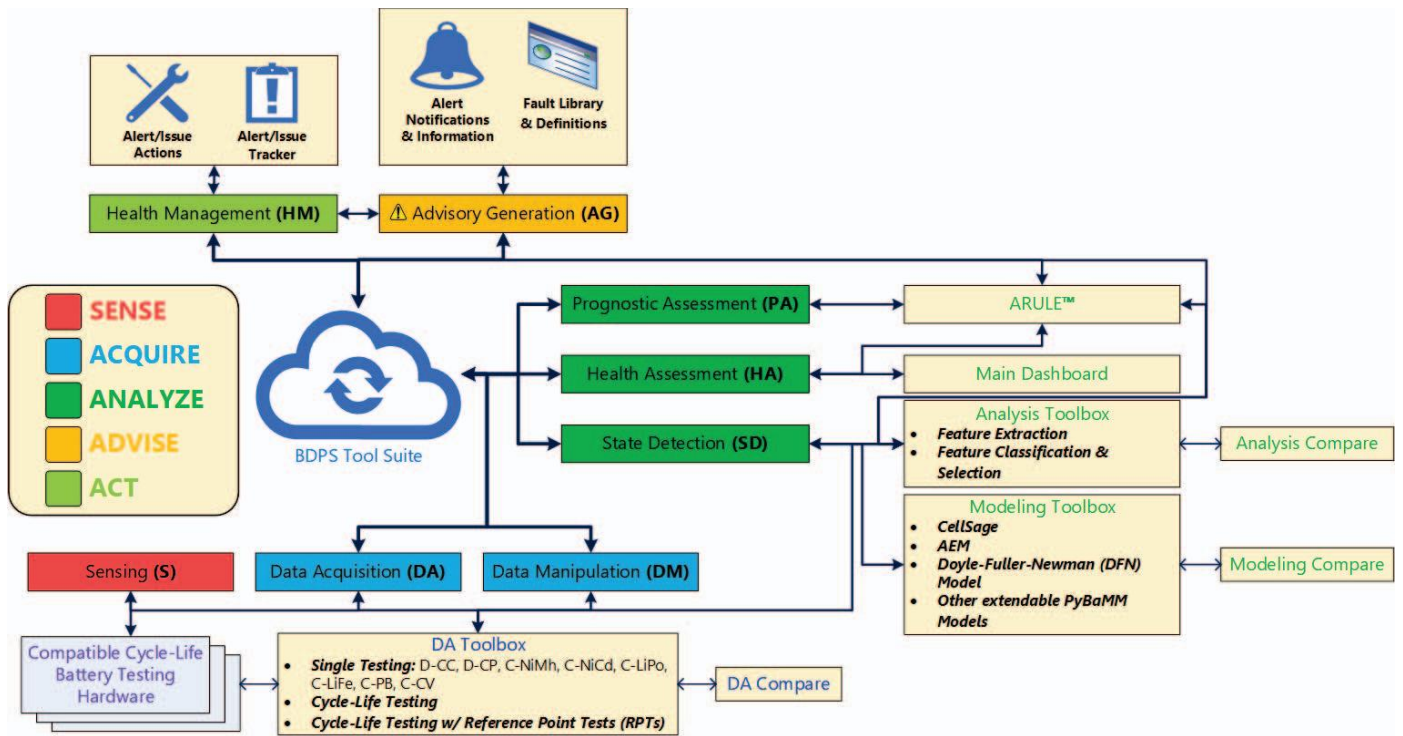


Figure 3. Functional Block Diagram of the BDPS Tool Suite relating it to the IEEE 1856-2017 PHM Standard.

Central to the DAQ subsystem's functionality is its proprietary Python-based control API, explicitly developed to control and manage serial data exchange with battery cyclers and microcontrollers. It facilitates automatic detection and connection of testing equipment via serial COM ports. Upon selecting the specific hardware from a predefined list within the GUI, users establish connections instantly, significantly reducing the complexity and time traditionally associated with configuring commercial battery cyclers. Once connected, the proprietary Python-based software continuously streams high-resolution battery cycling data—including voltage, current, temperature, and power—at a data acquisition rate of 1 Hz, achieving precision of 0.05% voltage accuracy (within 2.5–4.2 V) and current accuracy of ± 5 mA across a 0.05–10 A range. Data management forms another critical layer of the architecture. Raw cycling data, collected at 1 Hz, are systematically stored in structured CSV files for convenient retrieval and post-processing. Accompanying these datasets are detailed metadata records stored in JSON format, including critical hardware information (part numbers, accuracy, channels), testing parameters, and user-defined custom fields (such as cell fixtures or battery specifications). Data are securely synchronized both locally on the testing computer and remotely within a cloud-based storage system, offering scalable data accessibility and ensuring robust data integrity across multiple testing platforms.

The intuitive graphical user interface (GUI), another cornerstone of the DA Toolbox, supports comprehensive test programming functionality, real-time monitoring, and advanced data visualization. Users easily configure single (CC, CV, CP modes) or cycle-life with or without Reference Point Testing (RPT) charge/discharge protocols through the GUI, define cycling parameters including cutoff voltages, current ranges,

rest intervals, and number of test cycles. The GUI provides customizable graphical data visualization features enabling real-time plotting of critical metrics like voltage, current, capacity, and power versus time or cycle count. Users interact seamlessly with these graphs, overlaying multiple testing runs, zooming, panning, and exporting visualizations in industry-standard formats (CSV, PNG, PDF).

Data security and reliability are carefully considered throughout the BDPS architecture. Testing parameters are safeguarded through user credential authentication, and critical metadata—such as hardware identification details, test conditions, and configurations—are recorded and preserved meticulously in accompanying JSON files. Furthermore, the system continuously synchronizes data between local storage and cloud databases, ensuring redundancy and secure archival access.

III. INTEGRATING THE DA TOOLBOX WITH THE HIGH-LEVEL BDPS ARCHITECTURE

As illustrated in Figure 3, on a higher level, the BDPS architecture integrates several key components, with the DA Toolbox serving as the foundational subsystem. The diagram specifically highlights the DA Toolbox's role in interfacing the battery cyclers (bottom left) and batteries (top left) with the testing computer, which hosts the BDPS Tool Suite with cloud database (top right), facilitating a seamless data pipeline into the system's advanced modeling and analysis capabilities.

The DA Toolbox incorporates modular hardware interfaces, depicted in the battery cycler component, designed for compatibility with COTS battery testing equipment. These interfaces leverage serial communication via COM ports, as shown by the connection lines in the diagram, to link the cyclers

to the testing computer. The system also utilizes affordable microcontrollers to collect temperature data. This setup ensures that data from multiple battery test systems flows efficiently into the BDPS architecture. At the core of the toolbox is a proprietary Python-based control API framework, which manages data exchange between the cyclers and the testing computer, as reflected in the central data flow of Figure 3. This framework automatically detects and connects to available COM ports, recognizing compatible hardware from a predefined list via the GUI, streamlining setup compared to traditional commercial systems. Once connected, it streams high-resolution data—including voltage, current, temperature, and power—at a 1 Hz acquisition rate, achieving 0.05% voltage accuracy and ± 5 mA current precision. The data is stored in structured CSV files and accompanied by metadata in JSON format, capturing hardware details, test configurations, and user-defined fields. This data is synchronized securely to both local storage and the cloud database, as managed by the data analytics, prognostics, and informed decision-making component (bottom right), ensuring robust accessibility and integrity.

The DAQ Toolbox’s integration extends to the AEM, CellSage, and DFN component (middle right), where the collected data fuels advanced modeling and analysis. The high-fidelity DAQ outputs are compared against simulated benchmarked models such as the Doyle Fuller Newman (DFN) model, which simulates electrochemical processes like ion diffusion, charge transfer, and solid-electrolyte interphase (SEI) evolution, predicting internal states such as lithium concentration and overpotential. This data is also compared to CellSage simulations that model capacity fade, impedance growth, and thermal runaway risks, forecasting degradation under thermal stress (e.g., 75°C) or high-rate cycling (10C). Machine learning models, including Gradient Boosting Machines (GBM), Convolutional Neural Networks (CNN), and Recurrent Neural Networks (RNN) with attention mechanisms, utilize historical battery aging data (center) to predict remaining useful life (RUL), incorporating features like state of charge (SoC), internal resistance, and cycle asymmetry. Additional techniques such as Rate Capability Analysis (RCA) assess power delivery under varying discharge rates (e.g., 0.1C to 20C), while Voltage Relaxation Analysis (VRA) evaluates self-discharge rates post-rest, and Open Circuit Voltage (OCV) profiling tracks state of health (SoH) shifts with 99% correlation to reference measurements.

IV. TEST PLAN AND RESULTS

The testing was conducted using COTS EBC-A10H battery cyclers manufactured by ZKETech interfaced with ESP32/XIAO-nRF52840 microcontrollers. Each cycler is a single-channel device capable of precise control over current and voltage parameters, which is essential for cycle life testing accuracy. The test systems are connected to a dedicated computer interface as shown in Figure 1 for programming the cycling protocol and for real-time data acquisition, enabling automated tracking of each cell’s voltage, current, temperature, and capacity over every cycle. Battery specifications used for this test plan are as follows:

- **Battery Type:** 18650 lithium iron phosphate (LFP) cylindrical cells

- **Nominal Capacity:** 1.8 Ah
- **Initial Condition:** All cells were conditioned to have an initial capacity of 1.76 Ah before testing.

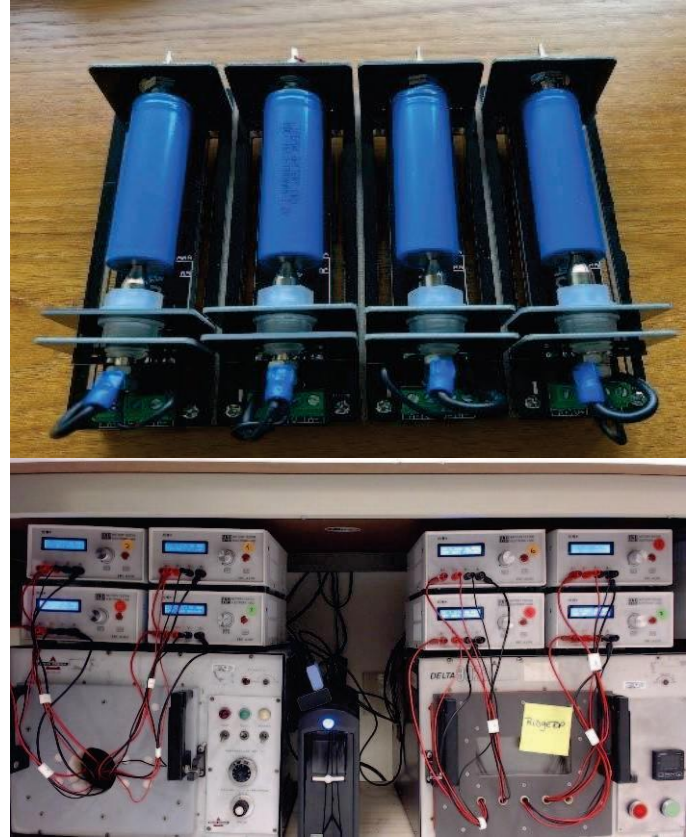


Figure 4. Experimental setup showing the batteries (top) and the cyclers with the thermal chambers (bottom).

The experimental setup was designed to accommodate eight batteries, divided equally between two temperature conditions. Each battery was connected to its own EBC-A10H cycler and microcontroller to allow independent cycling, ensuring consistency and isolation between test conditions. Four batteries were cycled at laboratory room temperature (20°C), while the other four were placed in a temperature-controlled chamber set to 40°C. This setup ensured that each cell was exposed to a stable and isolated thermal environment throughout the testing period. Temperature stability was monitored and maintained within $\pm 1^\circ\text{C}$ for both conditions to ensure precise control over the experimental parameters.

Figure 4 shows the experimental setup, with the batteries organized in separate areas to isolate the 20°C and 40°C temperature conditions. The figure also illustrates the connection of each battery to its corresponding EBC-A10H cycler and microcontroller. Batteries cycled at 20°C were positioned on an open laboratory bench, while those at 40°C were placed inside the thermal chamber. Each cell was securely clamped to ensure stable electrical contacts, and the chamber was equipped with thermocouples to monitor and regulate the temperature. This layout not only facilitated easy access to each battery for inspection but also minimized any cross-thermal effects between cells cycled at different temperatures. The cycle

life testing protocol applied the following steps in each cycle as shown in Figure 5:

- **Step 1:** Constant Current (CC) Discharge at 3C (5.4 A) until the voltage dropped to 2.5 V.
- **Step 2:** Rest period of 10 minutes following the discharge to allow for thermal and electrochemical stabilization.
- **Step 3:** Constant Current - Constant Voltage (CC-CV) Charge at 1.8 A until the cell voltage reached 3.65 V, followed by a Constant Voltage hold until the current tapered to 0.07 A.
- **Step 4:** Another rest period of 10 minutes following the charge phase.

This protocol was repeated for 600 cycles, simulating typical usage patterns for high-energy applications, to assess the cells' capacity retention under continuous cycling. The EBC-A10H cyclers provided real-time data logging for each cell, recording voltage, current, and capacity during each cycle. The initial capacity (1.76 Ah) was set as the baseline for tracking capacity fade over time. Capacity measurements were recorded periodically and analyzed to evaluate the rate of degradation across the two temperature conditions. Data were reviewed at regular intervals to assess trends in capacity fade and identify any potential anomalies.

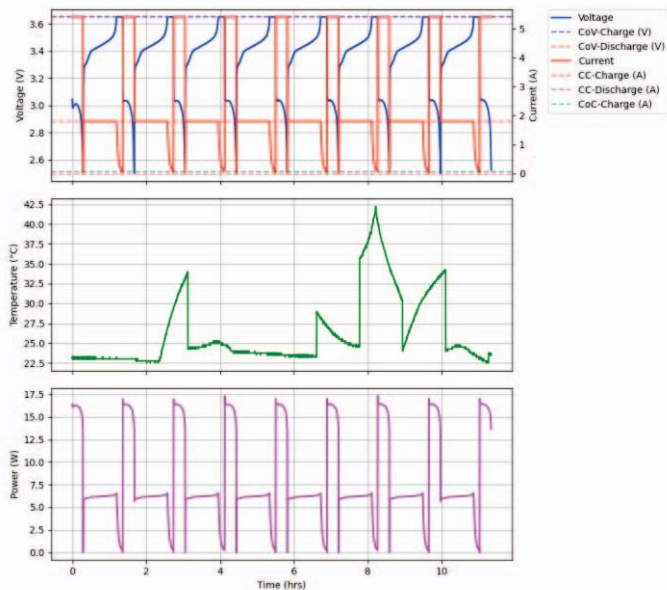


Figure 5. Testing results for the first 6-8 cycles. (Top) Voltage (blue) and Current (red) with thresholds: CoV-Charge (3.65 V), CoV-Discharge (2.5 V), CC-Charge (1.8 A), CC-Discharge (5.4 A), CoC-Charge (0.07 A). (Middle) Temperature. (Bottom) Power (Voltage \times Current). All plotted against hours elapsed.

At the start of testing, all 18650 LFP cells demonstrated a consistent initial capacity of approximately 1.76 Ah, providing a reliable baseline for assessing capacity retention across the different temperature conditions. Figure 3 shows the capacity data for the battery over different cycles. Over the course of 600 cycles, notable differences emerged between the cells cycled at

room temperature (20°C) and those at an elevated temperature (40°C), illustrating the impact of temperature on cycle life and degradation patterns in lithium iron phosphate batteries.

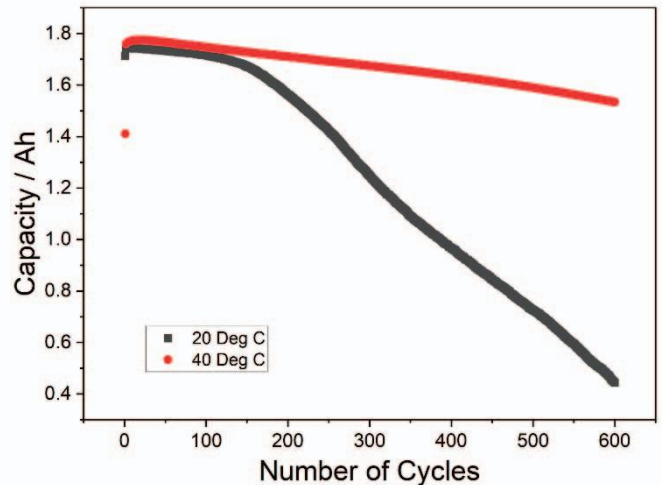


Figure 6. Capacity data over 600 cycles for two distinct temperatures: 20°C (black) and 40°C (red).

For the cells cycled at room temperature (20°C), capacity degradation was severe, with capacity dropping from 1.76 Ah to 0.4 Ah. In contrast, cells cycled at 40°C demonstrated a slower rate of degradation, with capacity only dropping to 1.5 Ah after the same 600 cycles. This outcome is somewhat surprising, as higher temperatures are generally expected to accelerate aging in lithium-ion cells due to increased reaction kinetics and potential electrolyte decomposition.

Several factors may explain this unexpected trend. For the cells cycled at 20°C, slower lithium-ion diffusion at this temperature could contribute to lithium plating during the CC-CV charge step, even at a moderate 1C charge rate. Lithium plating is more likely to occur as the battery nears full state-of-charge, especially in lower-temperature environments where ion mobility is reduced. Over many cycles, any plated lithium could become inactive, contributing to capacity fade.

Additionally, the continuous cycling at high discharge rates (3C) may induce mechanical stresses within the electrode material. At 20°C, these stresses could lead to microstructural changes, such as cracking or particle detachment, which would exacerbate capacity fade by impeding electron and ion transport pathways. In contrast, the elevated temperature of 40°C might allow for enhanced ion mobility and slightly better resilience to mechanical stress, thus reducing the severity of degradation over cycles.

The results suggest that for LFP cells under high-rate cycling protocols, elevated temperatures may unexpectedly benefit cycle life by reducing mechanical and electrochemical stress. This finding could have practical implications for battery management, suggesting that temperature regulation and cycling protocols should be optimized together to maximize battery lifespan in high-demand applications.

V. CONCLUSION

The BDPS Tool Suite, with its innovative Data Acquisition (DA) Toolbox, presents a transformative advancement in Prognostics and Health Management (PHM) for batteries by effectively integrating cost-effective hardware, proprietary Python-based communication protocols, and sophisticated data-driven degradation modeling. Through the development and validation of the low-cost DAQ Toolbox—which leverages proprietary Python-based serial communication to interface seamlessly with affordable cyclers such as the EBC-A10H—the BDPS significantly lowers financial barriers (below \$100/channel) while maintaining precision comparable to high-end commercial systems. The intuitive GUI facilitates scalable, user-friendly operation, ensuring robust data capture and comprehensive diagnostics across diverse operating scenarios. With proven accuracy in detecting critical degradation modes like lithium plating and capacity fade at an early stage, BDPS empowers small-scale researchers, startups, and industry professionals to proactively address safety, extend battery life, and optimize performance economically. As the demand for reliable and affordable battery management solutions escalates globally, the BDPS Tool Suite emerges as an essential platform, bridging accessibility with innovation, ultimately fostering a safer, more sustainable, and cost-effective battery ecosystem.

ACKNOWLEDGMENT

The authors would like to acknowledge xAI for their provision of Grok 3, an advanced AI model that has significantly supported the organization and formatting of this paper. We also extend our gratitude to the U.S. Department of Energy (DOE) for funding this project through SBIR Phase 1 Contract DE-SC0023738, which enabled the exploration and implementation of the technologies presented. Additionally, we appreciate the conversations with Martin Gauroy on his `zketch_controller` control code (https://github.com/GrizzlyFr/zketch_controller), which facilitated the integration of our battery cycler hardware with software.

REFERENCES

- [1] "IEEE Standard Framework for Prognostics and Health Management of Electronic Systems," in IEEE Std 1856-2017, vol., no., pp. 1-31, 13 Dec. 2017, doi: 10.1109/IEEESTD.2017.8227036.
- [2] Che, Y., Hu, X., Lin, X., Guo, J., & Teodorescu, R., "Health prognostics for lithium-ion batteries: Mechanisms, methods, and prospects.", *Energy & Environmental Science*, 16, 338–371. doi: 10.1039/D2EE03019E
- [3] Birkel, C. R., Roberts, M. R., McTurk, E., Bruce, P. G., and Howey, D. A., "Degradation diagnostics for lithium ion cells", *Journal of Power Sources*, vol. 341, pp. 373–386, 2017. doi:10.1016/j.jpowsour.2016.12.011.
- [4] von Bülow, F., Wassermann, M., and Meisen, T., "State of health forecasting of Lithium-ion batteries operated in a battery electric vehicle fleet", *Journal of Energy Storage*, vol. 72, Art. no. 108271, 2023. doi:10.1016/j.est.2023.108271.
- [5] Attia, P. M., Grover, A., Jin, N., Severson, K. A., Markov, T. M., Liao, Y. H., Chen, M. H., Cheong, B., Perkins, N., Yang, Z., Herring, P. K., Aykol, M., Harris, S. J., Braatz, R. D., Ermon, S., & Chueh, W. C. (2020). Closed-loop optimization of fast-charging protocols for batteries with machine learning. *Nature*, 578(7795), 397–402. doi: 10.1038/s41586-020-1994-5
- [6] Kumar, R. and Das, K., "Lithium battery prognostics and health management for electric vehicle application – A perspective review", *Sustainable Energy Technologies and Assessments*, vol. 65, Art. no. 103766, 2024. doi:10.1016/j.seta.2024.103766.
- [7] B. R. Das Goswami et al., "A combined multiphysics modeling and deep learning framework to predict thermal runaway in cylindrical Li-ion batteries," *J. Power Sources*, vol. 595, p. 234065, Mar. 2024, doi: [10.1016/j.jpowsour.2024.234065](https://doi.org/10.1016/j.jpowsour.2024.234065).
- [8] B. R. Das Goswami, Y. Abdisobbouhi, H. Du, F. Mashayek, T. A. Kingston, and V. Yurkiv, "Advancing battery safety: Integrating multiphysics and machine learning for thermal runaway prediction in lithium-ion battery module," *J. Power Sources*, vol. 614, p. 235015, Sep. 2024, doi: [10.1016/j.jpowsour.2024.235015](https://doi.org/10.1016/j.jpowsour.2024.235015).
- [9] B.R. Das Goswami, V. Jabbari, R. Shahbazian-Yassar, F. Mashayek, V. Yurkiv, "Unraveling Ion Diffusion Pathways and Energetics in Polycrystalline SEI of Lithium-Based Batteries: Combined Cryo-HRTEM and DFT Study," *J. Phys. Chem. C*, vol. 127, no. 45, pp. 21971-21979, Nov. 2023, doi: [10.1021/acs.jpcc.3c05395](https://doi.org/10.1021/acs.jpcc.3c05395).