NOVONIX

The Secret to Slashing Battery Test Times:

Ultra-High Precision Coulometry (UHPC) and Machine Learning

High resolution raw data, unique cycle metrics – UHPC has valuable applications in development, quality, and machine learning lifetime prediction.

Progress Demands **Urgency**

For any company dependent on the battery supply chain, whether sourcing cells for electric vehicles, qualifying novel materials or standing-up giga-factories, assessing cell quality, performance, and lifetime typically takes months to years of costly testing and is the single biggest bottleneck to energy storage innovation. But what if testing time was cut to a matter of weeks?

Degradation mechanisms in chemistries such as lithium-ion are non-trivial, often occurring at minuscule rates of reaction, making them difficult – or impossible – to capture on traditional spec cell testing equipment, requiring long-test times before differences are evident.[1,2] This is where techniques utilizing Ultra-High Precision Coulometry (UHPC) cell testing equipment excels, and data-driven predictive models thrive.

Filling the gaps between traditional cell testing and complex and/or destructive analytical techniques, UHPC offers quantifiable insights into electrochemical mechanisms which are otherwise invisible using other techniques. This article explores how cell and auto OEMs, materials companies, and world-class institutions use UHPC to cut an order of magnitude off their testing times, and how high-fidelity UHPC data unlocks opportunities for predictive Machine Learning (ML) methods.

UHPC: A Brief Background

UHPC was pioneered by Prof. Jeff Dahn in 2010 with the goal of accurately detecting low-rate electrochemical degradation in lithium-ion cells.[1,2] Since then, UHPC techniques have been published in hundreds of journal articles spanning many applications and chemistries. Prof. Dahn has primarily employed low-rate constant current cycling to accurately mitigate kinetic effects during cycling and accurately measure cycle metrics to correlate to long-term performance. However, a boundless list of techniques can benefit from the use of UHPC across the development lifecycle, from fundamental material synthesis work to quality control in mass manufacturing. In 2013, following industry-wide demand for commercial cell testing equipment capable of UHPC techniques, Dr. Chris Burns and Dr. David Stevens, both mentored by Prof. Dahn, founded NOVONIX and commercialized the first market-ready UHPC cell testing product, which has evolved and spread across the battery industry over the last 12 years.

UHPC equipment requires the highest precision and accuracy possible to allow researchers to develop methods to understand specific electrochemical degradation mechanisms during cell testing and measure metrics such as coulombic efficiency accurate to 10s of ppm. These mechanisms involve cell materials such as anodes, cathodes, electrolytes, etc., exchanging electrons at electrode surfaces in complex reactions. As degradation occurs, the associated processes which create charge balance in the cell while undergoing testing cause tiny differences in charge and discharge capacity.

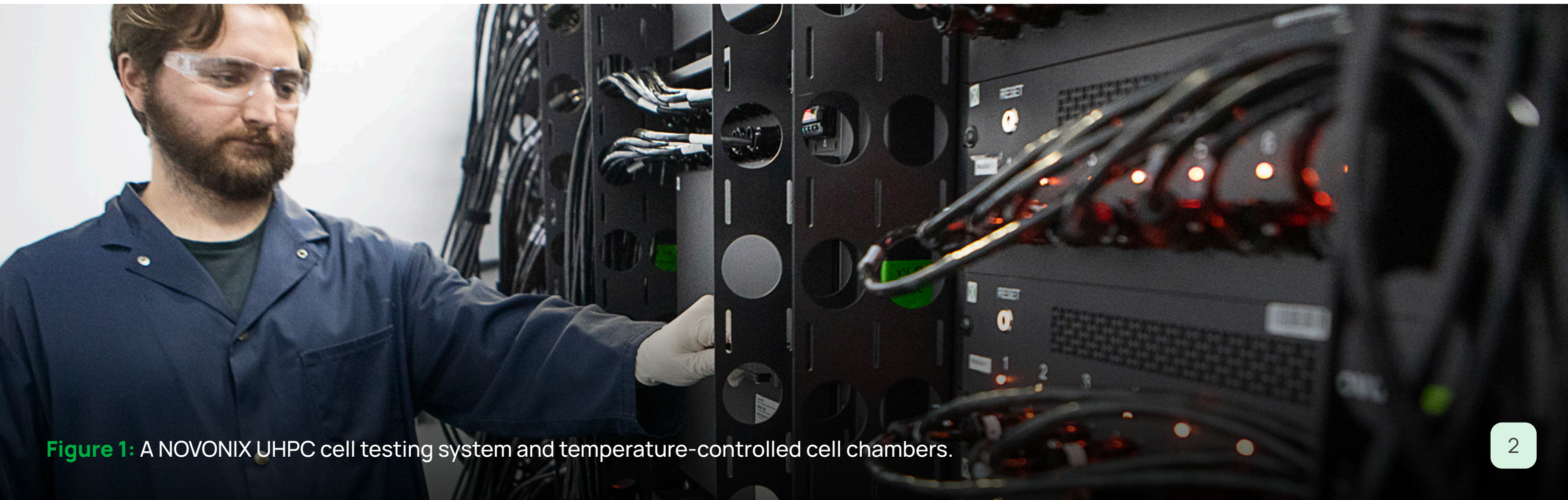


Figure 1: A NOVONIX UHPC cell testing system and temperature-controlled cell chambers.

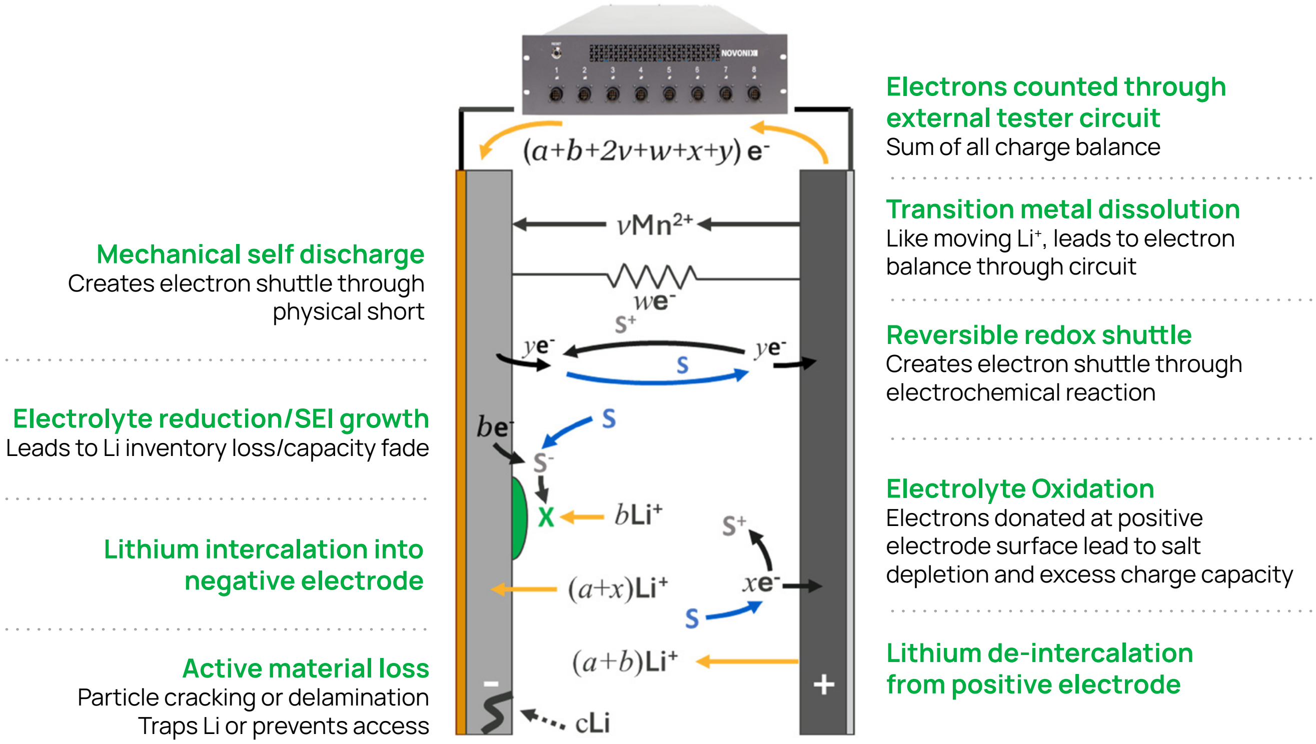
These processes are shown in Figure 2 and include, but are not limited to:

- Electrolyte reduction and oxidation
- Transition metal dissolution
- SEI formation
- Mechanical self-discharge
- Active material loss/particle cracking
- Reversible redox shuttles

UHPC data can add a previously unattainable level of insight into cell chemistry and processes leading to end of life. These data therefore have important implications in the field of predictive analytics for batteries.

Figure 2: Electrochemical degradation and charge balance mechanisms occurring during a charge cycle of a lithium-ion cell.

Charge Balance Mechanisms During Cell Testing



To create charge balance in a cell during testing, electrons and ions must be exchanged in every electrochemical reaction. These processes can add capacity during charge and subtract capacity during discharge, all contributing to the Coulombic Efficiency.

Learn more about UHPC – Volta Foundation Battery Forum: Supercharging Battery Development with UHPC

Battery Failure Prediction

A variety of methods are used to predict the lifetime of cells under various conditions. These include:

- Empirical aging models
- Qualitative ranking
- Physics-based models
- Machine learning

Each method has advantages and disadvantages. For example: empirical models can be iterated quickly but do not generalize well, qualitative ranking provides a holistic picture of cell degradation but requires subject-matter expertise and excessive time, physics-based models give detailed performance predictions but require extensive parametrization, and ML models provide broad predictions at low cost but typically require large training data sets.

UHPC is historically reported in the literature adopting qualitative approaches, making head-to-head comparisons of similar systems such as different electrolyte additives in the same cells, comparisons of electrode materials, or direct measurements of specific mechanisms such as lithium plating or self-discharge.[3-5] However, the insights from UHPC can complement other modeling methods such as ML and may pave a way for more accurate prediction capabilities.

There is often a strong correlation between early electrochemical signatures and eventual cell failure.[6] ML models thrive on exactly the kind of high-resolution UHPC data that captures those first, almost imperceptible signs of degradation. By training models on thousands of cells whose subtle early-cycle fingerprints are paired with their eventual end-of-life metrics, models can learn to map “day-one” electrochemical features to long-term performance outcomes. This ability to forecast lifetime after only a handful of cycles can shorten qualification and validation loops from months-years to days-weeks and turn UHPC into a launchpad for data-driven battery R&D.

> Figure 3 depicts one method of how UHPC could be used for ML lifetime prediction. This method was employed during the case-study in this article.

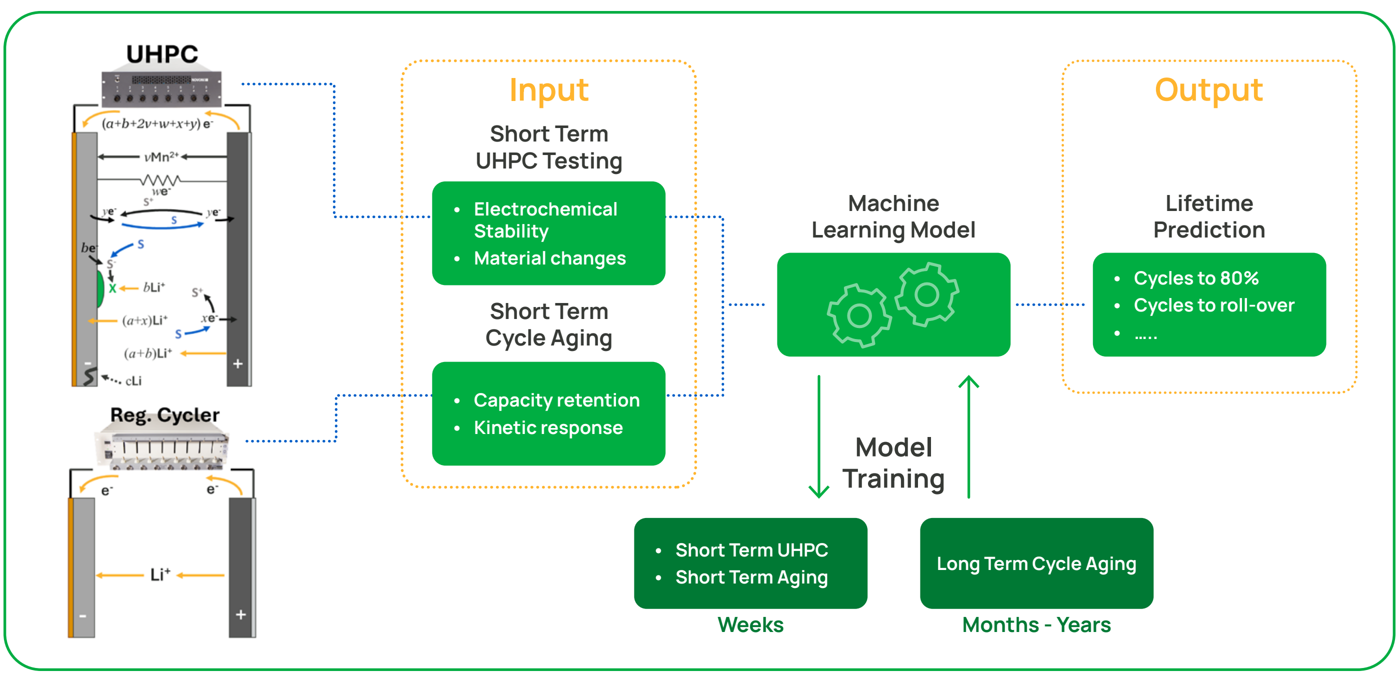
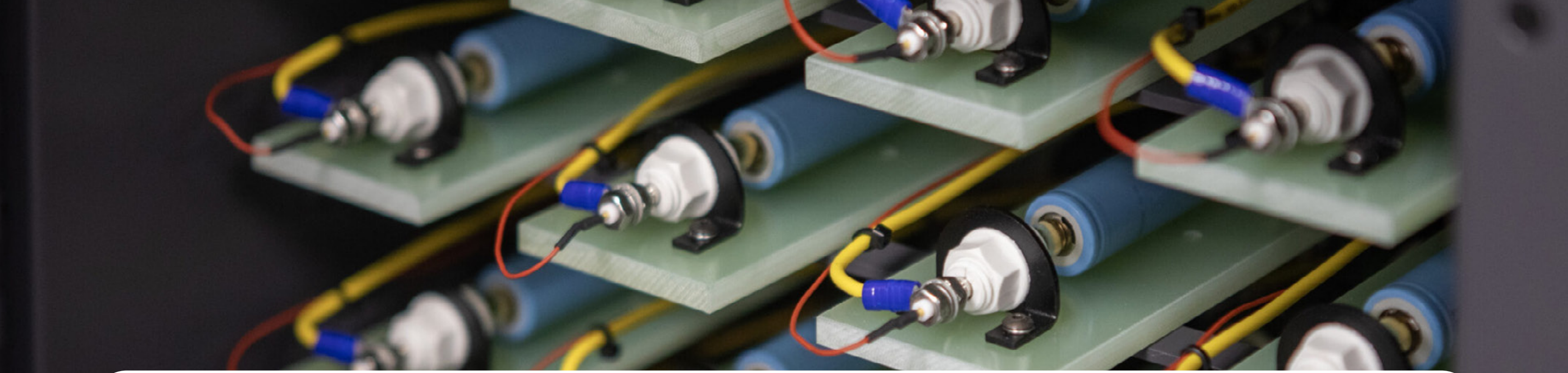
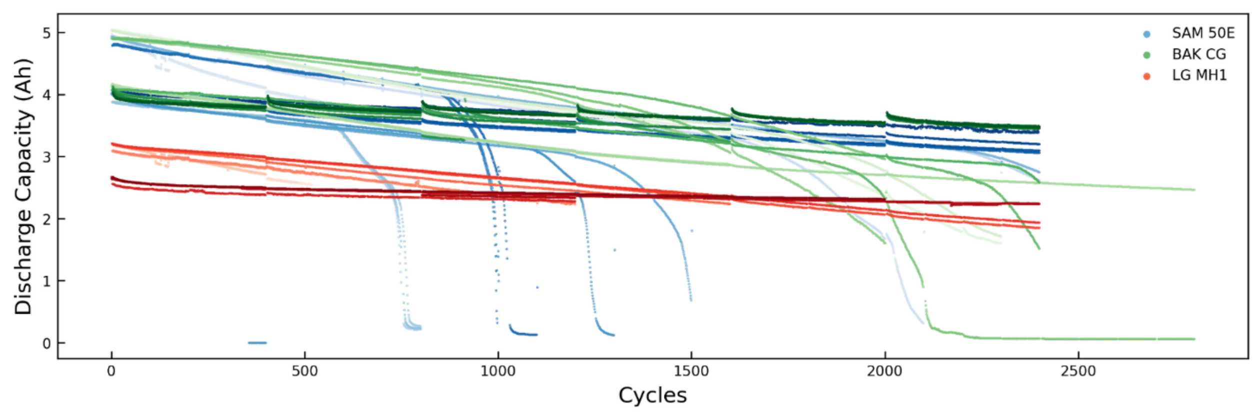


Figure 3: Model diagram for lifetime prediction model using short term UHPC and short-term cycle data trained on paired UHPC and long-term cycling results.

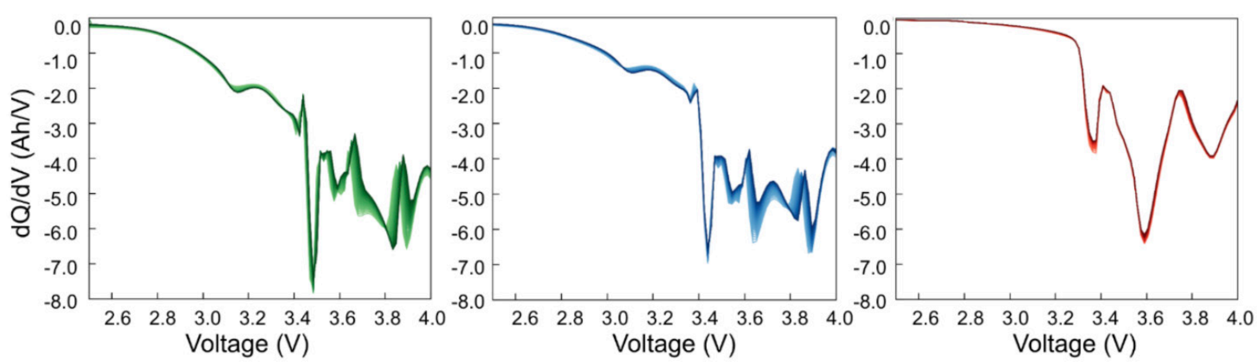


UHPC and ML: A Case Study

A recent study performed by NOVONIX and SandboxAQ demonstrated the potential value of UHPC for ML cell cycle life predictions. The goal was to develop a model that was generalizable across various degradation signatures based on approximately 1 month of UHPC testing.



Cycle life curves from standard R&D systems over nearly two years of testing. Three cell types were tested at various temperatures and cycling voltages leading to varied degradation signatures. This controlled data set generation strategy was used as a baseline to develop UHPC-resolved features for ML Models



Representative UHPC differential capacity curve evolution over 50 cycles for the three cell types considered. Each tuple (cell type, temperature, and voltage) I underwent both long-term and UHPC testing. The UHPC data was then used for predicting cycle life to target capacity retention.

Figure 4: Cycle life trajectories for three cell types tested at various temperatures and voltages (top). UHPC discharge differential capacity profiles for each cell type at a single temperature and voltage range (bottom).

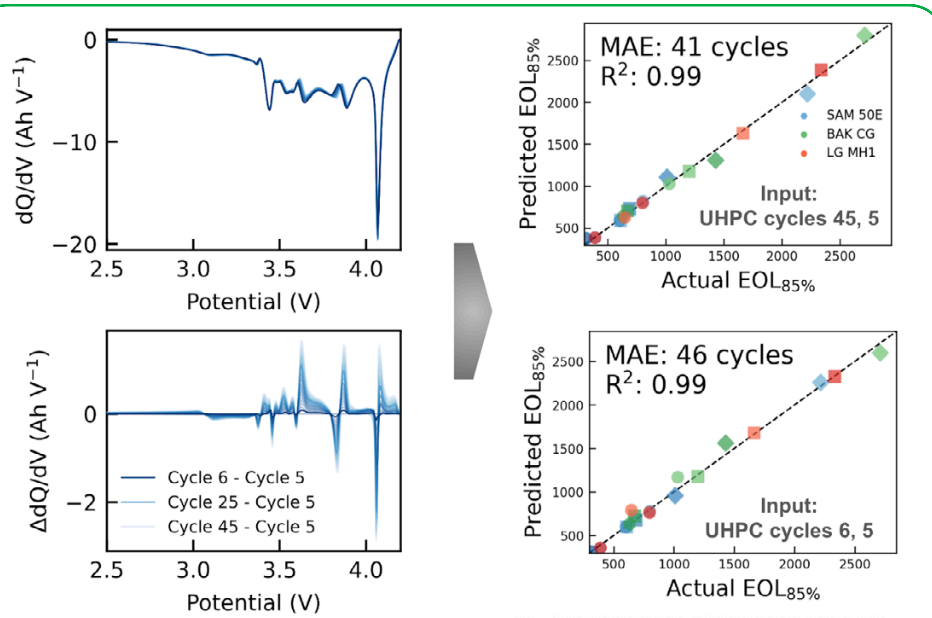
Cylindrical cells from three manufacturers were tested using various voltage ranges and temperatures. All cells contained high-Ni positive electrodes, two types contained silicon-graphite blend negative electrodes, and one cell type contained a graphite-only negative electrode.

Testing conditions were selected to cover specific degradation mechanisms based on the known cell compositions:

- Cells with Si-containing negative electrodes were tested to full DOD and ~70% DOD to isolate Si-related degradation.
- All cell types were tested to 4.06 V and 4.2 V to isolate degradation due to highly delithiated high-Ni positive electrode materials.
- Cells were tested at 25°C, 40°C, and 60°C to account for degradation temperature dependence.

Cells were cycled in triplicates for each test condition (cell type, temperature, voltage range); on a NOVONIX UHPC system at C/10-C/10 constant current cycling for approximately 4 weeks, and on a common R&D-spec system for up to 2500 cycles (~2 years) at C/3-C/3 (CCCV charge to C/20).

The capacity retention of long-term cycling data was used as the target metric for ML predictions. Various capacity retention thresholds were considered, for example 90%, 85%, and 80%. To construct features that capture cell degradation, residuals of differential capacity (dQ/dV) curves between two cycles were computed from the paired UHPC data. Figure 5 shows that using merely 6 UHPC cycles, the number of cycles to 85% capacity retention was predicted to be within 46 cycles for cell types not used in model training. These results are a dramatic improvement over traditional methods used in the literature, such as early discharge capacity trends and changes in low resolution voltage features.[6-8]



UHPC-resolved residuals between two discharge differential capacity curves provide the input to construct electrochemically meaningful features for ML models.

Cycle life predictions on a cell type left out from model training. Three separate models are shown, each trained on two of the three cell types. UHPC-resolved features enable generalizable cycle life predictions.

Figure 5: Machine learning feature engineering approach. Discharge differential capacity (dQ/dV) curve residuals between two cycles are used to construct electrochemically meaningful features (left). Model cycle life predictions using 45 UHPC cycles (top right) and 6 UHPC cycles (bottom right).

Ultra-High Generalization

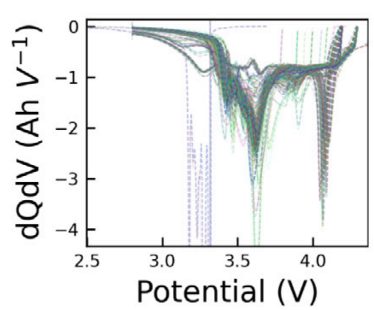
How well can UHPC-derived features generalize to arbitrary data sets? The same features described above, developed on a small, curated data set were directly applied to a data set of over 4000 cells composed of various chemistries, including both Ni-based and LFP positive electrodes, and graphite and silicon-containing negative electrodes, from a variety of vendors. Each testing condition contained UHPC/long-term paired cells. The same ML pipeline described above was applied to this data set, with features constructed from the residual UHPC differential capacity curves.

By directly applying the ML feature generation approach developed on a small, curated data set to a data set 100 times larger, with merely 25 UHPC cycles as input, the number of cycles to 85% capacity retention was predicted to within 108 cycles.

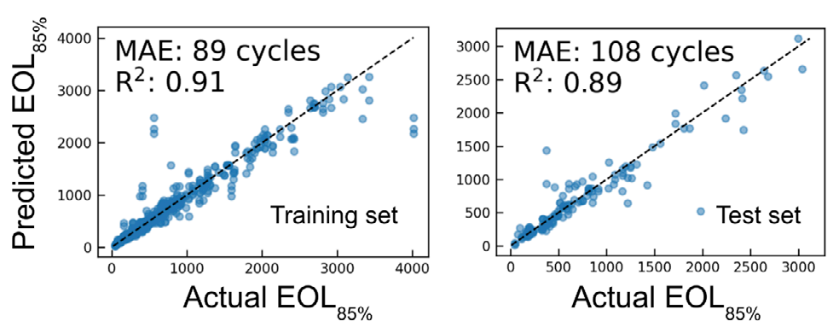
The success of this method to generalize arbitrary data sets is due to how electrochemical processes that lead to cell degradation over a long-time scale can be encoded in early-life features with high-fidelity data. The precision and accuracy of UHPC makes this ML approach possible.

Although this methodology shows great promise for generalizable accurate lifetime prediction, some limitations exist or were not investigated in this case-study. For example, the data shown in this study was all obtained from “fresh” cells (i.e. no previous testing after formation). Cells with varying or unknown age or history could not be used with the same ML model, since the model was trained with cells of a specific history. Typically these types of limitations exist in ML models: previously unseen conditions will perform poorly. Other causes of performance limitations and outliers, including those in this study, may occur due to data sets with few dQ/dV features such as LFP or high-silicon containing cells, narrow test conditions in the training set, and poor training data (perhaps due to poor quality cells, poor temperature control in cycle aging, etc.).

There also exist methods to improve these models, such as more robust training sets with broader test conditions, more cell chemistries, or by generating more electrochemical or physics-informed features to train in the models such as impedance via Direct Current Internal Resistance (DCIR) or Electrochemical Impedance Spectroscopy (EIS), as well as UHPC cycle metrics such as coulombic efficiency, charge-endpoint capacity slippage, and capacity fade.



UHPC differential capacity curves from over 2000 cells from various vendors. Cell differences include electrode chemistries and morphologies, form factors, and electrolyte compositions.



Cycle life predictions using UHPC-resolved features from differential capacity residuals. 10 % of the data was held out from model training to test predictions. These results demonstrate the utility of combining UHPC with ML.

Figure 6: UHPC discharge differential capacity (dQ/dV) curves for over 2000 cells from various vendors (left). Cycle life predictions for a model trained using features from differential capacity residuals (right).

The Future of Battery Testing

The results shown in this article have important implications on all aspects of battery development and commercialization, spanning material evaluation to warranty estimation. Utilizing UHPC channels to complement a suite of standard cyclers can significantly impact decisions and progress using short-term, high-throughput precision tests and predictive analytics. New measurement techniques and equipment in combination with advancements in ML and AI have significant implications for the battery lab of the future. Paired with proper data aggregation, labeling, and organization, investments in R&D will go further and faster. This is precisely why NOVONIX has focused on commercializing this technology with top-of-the-line equipment to offer higher fidelity learning for resource-limited teams. NOVONIX offers UHPC testing equipment capable of as low as nA resolution up to 20A-capable channel modules and chambers.

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Author Bios

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