Evaluation of Accuracy for Automated Method of Predicting Capacity Loss in Li-Ion Batteries

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***Abstract*— This paper provides an overview, methodology, and accuracy assessment detailing the collaborative efforts between Ridgetop Group Inc. (Ridgetop) and Idaho National Laboratory (INL) in advancing the system architecture of the CellSage battery health modeling, simulation, and analysis software platform to allow end users to adapt the CellSage battery modeling tool to make predictions for batteries for which an end user has necessary baseline cycle life and calendar life aging data. These efforts resulted in the design and development of automated regression analysis methods for baseline battery aging data, aiming to extract essential model parameters for Sigmoidal Rate Expressions (SREs). Such SRE parameters are utilized in CellSage to predict battery aging under reasonable use, such as arbitrary conditions of temperature, state of charge, and other operating conditions related to a specific battery duty cycle. The underlying technology core is based on a patented approach where the sum of SREs has been demonstrated to accurately model the loss of lithium inventory (LLI) and loss of active material (LAM) as the dominant aging mechanisms within lithium-ion batteries. Throughout this paper there is a discussion on various types of battery State-of-Health (SoH) Prediction models, an overview of how capacity loss is calculated with SREs, and a comparative analysis that evaluates the accuracy of the new automated regression analysis methods for eight baseline aging datasets from various battery chemistries and cell types.**

Keywords— Batteries, Modeling, Simulation, Prognostics, Predictive Analytics

I. Introduction

Battery health modeling, simulation, and analysis play a crucial role in predicting the performance and longevity of lithium-ion batteries in diverse applications ranging from consumer electronics to electric vehicles. This paper presents a collaborative initiative between Ridgetop Group and Idaho National Laboratory aimed at enhancing the CellSage battery health modeling software. CellSage is a collection of patented modeling tools that enable diagnostics and predictive evaluations of battery life and mission readiness. Through the U.S. Department of Energy (DOE) Office of Technology Transitions, Ridgetop Group has partnered with INL to license, enhance, and commercialize this technology for battery manufacturers, researchers, and integrators on a global scale. Ridgetop and INL have been working together since 2015, but the primary focus of the collaboration highlighted in this paper was to overcome limitations associated with the original method of extracting model parameters from historic baseline aging data and develop automated regression analysis methods that could be deployed in a standardized graphical user interface (GUI). These advancements were integral to addressing several challenges posed by the previous method, including the reliance on third-party software and the lack of a standardized curve fitting approach across all baseline aging datasets.

The modifications to the CellSage system architecture aim to enhance user adaptability, allowing end users to leverage predictive capabilities for batteries with relevant baseline aging data. The development of automated regression analysis methods simplifies the extraction of essential model parameters, specifically for the Sigmoidal Rate Expressions (SREs). This updated approach permits the storage and GUI editing of each SRE parameter in a dynamic cell chemistry library, promoting flexibility for parameter updates. By eliminating the reliance on third-party software and incorporating user-friendly features, the enhancements result in significant cost and time savings, streamlining the previously laborious process of manual regression analysis and hard-coding or resulting simulation parameters.

The absence of a standardized curve fitting approach in the previous method has also been rectified, ensuring that results are not hard-coded to remain within boundary conditions. The updated methodology also minimizes the prerequisite for an in-depth understanding of battery aging, electrochemistry, and the intricate details of the underlying SRE modeling approach. This feature also enhances the usability of CellSage, making it more widely applicable across different user backgrounds and expertise levels.

The subsequent sections of this paper shall cover the methodology employed in developing two distinct automated regression analysis methods, the calculation of capacity loss using SREs, and a comprehensive comparative analysis that assesses the accuracy of these new methods across eight baseline aging datasets representing various battery chemistries and cell types. Through these discussions, we aim to demonstrate the robustness and versatility of the enhanced CellSage platform in predicting battery aging under diverse operating conditions.

II. Different Types of Battery SOH Prediction Models

Battery State-of-Health (SOH) estimation is a critical aspect in the performance and management of modern lithium-ion

batteries. Accurate assessment of SOH is essential for optimizing battery life, ensuring safety, and enhancing overall efficiency. Throughout the last several decades, various methodologies have been developed to estimate battery SOH, each leveraging different principles and techniques. This paper provides an overview of five distinct types of battery SOH estimation methods as highlighted in several recent publications: Empirical and Equivalent Circuit Models, Purely Data-Driven Models, Physics-Based Models, Purely Artificial Intelligence (A) and Machine Learning (ML) Models, and Hybrid Models. [4][5][6][7]

A. Empirical and Equivalent Circuit Models:

Empirical models are based on experimental data and statistical analyses. These models often use regression techniques to correlate observable parameters, such as voltage and current, with the battery's degradation over time. Equivalent circuit models, on the other hand, represent the internal behavior of a battery using electrical components like resistors and capacitors. Combining empirical data and equivalent circuit models allows for a good starting point to understand battery behavior and degradation mechanisms. However, this modeling approach is subject to known limitations such as limited accuracy, parameter sensitivity, and minimal prediction capabilities in the absence of electrochemistry, physics, and thermodynamics.

B. Purely Data-Driven Models:

Purely data-driven models rely on machine learning algorithms to analyze large datasets and identify patterns related to battery degradation. These models do not necessarily incorporate physical principles governing the battery's operation but are effective in capturing complex relationships within the data. Common techniques include neural networks, support vector machines, and regression models trained on historical data to predict future SOH.

C. Phyiscs-Based Models:

Physics-based models leverage knowledge of the underlying physical and chemical processes within a battery. These models consider factors such as electrode kinetics, thermal effects, and electrochemical reactions to simulate the battery's behavior. Physics-based models provide a deep understanding of the fundamental mechanisms governing battery degradation, making them valuable for accurate SOH estimation in various operating conditions. The core architecture within CellSage consists of physics-based models. After calibration with baseline aging data, CellSage is able to forecast deviations from baseline aging under various user-defined operating conditions. This capability provides a solid foundation for evaluating the aging effects under virtually limitless combinations of battery use conditions.

D. Purely AI and ML Models:

Purely AI and machine learning (ML) driven models are designed to capture intricate patterns and relationships within battery datasets without explicitly relying on physical principles. These models, including deep learning architectures like neural networks, use complex algorithms to uncover hidden features in the data and predict the SOH. Purely AI and ML models are particularly effective when dealing with non-linear and dynamic relationships in large datasets.

E. Hybrid Models:

Hybrid models combine the strengths of both physics-based and data-driven approaches. By integrating physical principles with machine learning algorithms, hybrid models aim to improve accuracy and robustness in SOH estimation. These models capitalize on the interpretability of physics-based models and the pattern recognition capabilities of machine learning, resulting in a comprehensive framework suitable for various battery types and usage scenarios. This approach has also been applied at INL where the research team evaluated a three hybrid modeling methods that combined the physics-based SRE foundation in CellSage with predictive curve-fitting (CF), ML, and Deep Learning (DL) methods coupled with Monte Carlo simulation. As reported in a recent Cell Press article, this method demonstrated that just 2-3 weeks of testing data on battery capacity loss could accurately predict capacity loss 8-12 weeks ahead. For many test cases the relative error rate was 5%-10% and the absolute error rate was 1%-2%. [2]

Understanding and accurately estimating the SOH of batteries are crucial for the widespread adoption and deployment of lithium-ion batteries for targeted applications such as electric vehicles, grid energy storage, and consumer electronics. The choice of the most suitable method depends on factors such as available data, computational resources, and the desired balance between accuracy and interpretability. Researchers and practitioners can benefit from this comprehensive overview to make informed decisions when selecting and implementing battery SOH estimation methods and capacity fade models for various applications.

III. Predicting Battery Capacity Loss Using Sigmoidal Rate Expressions for LLI and LAM

CellSage utilizes Sigmoidal Rate Expressions (SREs) to calculate battery degradation and provide predictions for both cycle life and calendar aging. As proven by INL in multiple research publications [1][2][3], the fundamental idea is that the reduction in overall battery capacity is influenced by prevailing aging mechanisms, notably Loss of Lithium Inventory (LLI) and Loss of Active Material (LAM), which can be accurately modeled with SREs. In some cases, there is an additional mechanism that emerges due to excess lithium that is released from the cathode as it slowly undergoes thermodynamic re-stabilization of its crystalline form, wherein a capacity gain is observed and can also be modeled using an SRE.

In the context of battery systems, SREs function as a chemical engineering tool, effectively describing the evolution of detrimental chemical reactions and other degradation processes (e.g., mechanical degradation of electrode materials) and their consequences within a batch reactor containing multiple aging mechanisms. This concept can be expressed mathematically as shown in Equation 1 on the following page.

$$Capacity\ Loss\ = \qquad (1)$$

$$\sum_{i=0}^{z} M_0 + 2(M_i - M_0) * \left[\frac{1}{2} - \frac{1}{(\,1 + \exp((a_i t)^{b_i}\,])}\right]$$

Each SRE encompasses three distinct physical parameters denoted as 'a,' 'b,' and 'M,' collectively portraying the evolution of a specific aging mechanism either over time or through cumulative battery cycles. These three parameters capture chemical kinetic and thermodynamic information about each aging mechanism. The maximum extent of capacity loss due to the i^{th} mechanism is given as M_i. The rate constant for the i^{th} reaction is given as a_i. Finally, the order of reaction of the i^{th} reaction or process is given as b_i. Time is represented by t. Note that the total sum if M_i terms should reside within 0 to 100% relative to pristine capacity at beginning of life (BOL).

When applying SREs to regress aging data, such as the percentage of capacity loss as a function of time, it is necessary to adhere to certain guidelines in order to obtain physically meaningful values of the SRE parameters M_i, a_i, and b_i. All values of M_i, a_i, and b_i are greater than zero. The maximum extent and rate of the i^{th} reaction, given as M_i, and a_i, respectively, ought to increase with increased stress factors: higher temperature, greater relative charge (higher SOC), greater depth of discharge, and higher charge and discharge current. The order of reaction of the i^{th} reaction, b_i, indicates whether the reaction is a surface (LLI) or volume (LAM) process. Finally, the battery cannot lose more than 100% of pristine capacity, thus the sum of the extent of reactions must be less than 100%; $\sum_{i=0}^{N_R} M_i \leq 100\%$, where N_R represents the number of reactions considered by the sum of sigmoids. These restrictions are summarized in *Figure 1*.

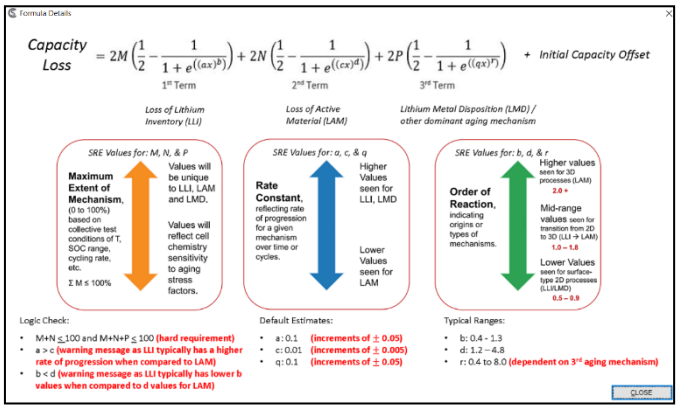

Figure 1: Description of SRE parameters for modeling capacity loss in CellSage

As determined through regression or other means, the SRE parameters M_i, a_i, and b_i are functions of specific battery chemistry And use conditions as detailed above, making the SRE parameters a unique thumbprint of aging for a chosen cell chemistry under specific use. As such, they provide a foundational physics-based framework for categorizing aging responses. Consequently, they can be employed to reveal insights into (1) improvements in cell chemistry and (2) alterations to cell usage conditions that could mitigate the rate and extent of aging. In practice, CellSage adapts the SRE parameters toward specific use conditions that may well vary over the timeline, providing an ideal platform for investigating *aging path dependence*.

As shown in the recent Cell Press article [2], the utilization of SRE-type expressions is gaining recognition as an effective predictive tool for describing battery aging behavior. This positive trend indicates a shift toward embracing physics-based methods and reducing reliance on empirical mathematics.

SRE modeling is pivotal for comprehending the aging process of lithium-ion batteries. As battery energy storage (BES) gains traction in sectors like electric vehicles and stationary energy systems, it becomes imperative to implement advanced battery management systems (BMS) that can compare real time degradation data against proven physics-based models like CellSage. When fully integrated, such BMS designs enable real-time monitoring of battery health, prediction of aging trends, and early detection of potential failures during operation. This proactive approach enhances battery longevity and contributes to safety and sustainability, aligning with the ongoing shift towards electric solutions aimed at achieving zero emissions.

Understanding the root causes of degradation is vital for guiding improvements in battery chemistry and corrective strategies. Battery aging is influenced by factors like path dependence, cell chemistry, and the differentiation between reversible and irreversible performance losses. To address these complexities, Ridgetop and INL researchers have collaborated extensively to test and validate the SRE modeling approach within CellSage to allow for the identification and classification of aging modes using electrochemical data.

IV. Automatic Regression Analysis to Extract SRE Model Parameters

It is possible for a CellSage user to adapt the battery-modeling tool to model battery capacity loss for a battery of interest. To do this, it is necessary to determine calibration parameters from four specific datasets: two datasets with measured aging that occurred during cycle testing at different temperatures and all other variables the same between the two measurements, and two datasets with measured aging that occurred during calendar testing at different temperatures and all other variables the same between the two measurements. These datasets are imported into the chemistry-import feature via the GUI shown as Figure 2.

The top-right corner of Figure 2 shows the sum of sigmoids used to model battery capacity loss in CellSage, and is shown as Equation 1. The central-right region of Figure 2 shows cycle-life capacity loss data (dotted line), the corresponding fit achieved with the non-linear least squares method of fitting (solid purple line), and the mechanisms of loss associated with LLI, and LAM as green and blue dashed lines, respectively. Fitting parameters determined by the non-linear least squares curve-fitting algorithm are shown below the plot of the associated curve fit and mechanistic components.

Figure 2: CellSage New Chemistry Import Feature.

Temperature parameters associated with the four datasets are automatically calculated after each dataset has been fit with the user-selected two or three-term SRE model. Given the two datasets per capacity-loss mode (either cycle-life capacity loss, or calendar-life capacity loss), activation energy is calculated according to Equation 2.

$$E_a = \frac{RT_1T_2}{T_2 - T_1} \cdot \left(\ln\left(\chi(T_2)\right) - \ln\left(\chi(T_1)\right)\right) \quad (2)$$

Activation energy of parameter χ, where χ is the parameter whose activation energy is being calculated, is given by E_a, the ideal-gas constant by R, and absolute temperatures of experiment 1 and experiment 2 by T_1 and T_2, respectively. Activation energy is calculated according to Equation 2 for each parameter determined with the non-linear least squares curve-fitting process.

Equation 2 was determined assuming $\chi(T_1)$ and $\chi(T_2)$ were determined as parameters from the fitting process. If the parameter χ follows the Arrhenius rate law, then $\chi(T_1) = \chi_0 \cdot \exp(-E_a/RT_1)$, and $\chi(T_2) = \chi_0 \cdot \exp(-E_a/RT_2)$, where χ_0 is the value of χ at infinite temperature. Taking the natural log of each equation gives $\ln\left(\chi(T_1)\right) = \ln(\chi_0) - E_a/RT_1$ and $\ln\left(\chi(T_2)\right) = \ln(\chi_0) - E_a/RT_2$. If the activation energy and parameter value, χ at infinite temperature are the same for each temperature, then subtraction of the natural log of the two parameters given $\ln\left(\chi(T_2)\right) - \ln\left(\chi(T_1)\right) = E_a(1/RT_1 - 1/RT_2) = E_a((T_2 - T_1)/(RT_1T_2))$. Solving the previous for E_a gives Equation 2.

Fitting results and regression efficiency are dependent on initial estimates of the SRE parameters. Users can either estimate these initial parameter values by visually analyzing the dataset or utilize an initial estimate provided through the genetic-algorithm fitting method detailed below. Additionally, any number of parameter values, from zero to one less than the total number of parameters of the model used to fit data can be fixed by the user. This flexibility proved essential because the parameter space defined by the capacity-loss model spans either six or nine dimensions, whereas many capacity-loss datasets often lack the total number of test cycles necessary to observe the maximum extent of LLI and LAM. Consequently, the ability to fix a parameter can significantly reduce the total parameter space from six or nine dimensions down to as little as one dimension.

Consider the genetic algorithm employed for generating initial estimates of SRE parameters within the CellSage capacity-loss simulation model. As covered in the previous section, CellSage utilizes a combination of two or three sigmoid functions to depict battery capacity loss under realistic, arbitrary usage scenarios. The calibration process of CellSage necessitates the computation of either six or nine SRE parameters. Identifying the optimal set of SRE parameters can pose challenges, as local extrema within the parameter space may cause algorithms such as the Levenberg-Marquardt method to become trapped in these local extrema. Unlike methods reliant on derivatives, such as the Levenberg-Marquardt method, a fitting approach like the genetic algorithm is less prone to converging towards a solution associated with a local extremum.

Conceptually, the genetic algorithm works according to Figure 3.

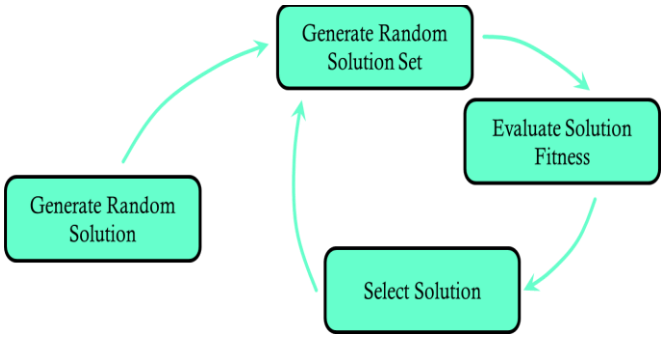

Figure 3: Genetic algorithm

The genetic algorithm as implemented for CellSage begins by generating a random set of three values for each of the six or nine SRE parameters, depending on whether the two or three-term model is selected for fitting the data in question. The chosen model is evaluated using exhaustive combinations of the randomly-generated possible solutions.

The solution with the best fit is determined according to the sum of squares error and whether or not the following restrictions are met by the proposed solution: the sum of the maximum extent of each reaction is less than 100%; the rate of reaction of LLI must exceed the rate of reaction LAM; the order of reaction of LLI must be less than the order of reaction of LAM; the ratio of the extent of LLI to LAM must be greater than 0.325 and less than 3.0; the magnitude of the LLI rate constant must be sufficiently close to 0.1; the value of the LAM rate constant must be sufficiently close to 0.005; the LLI order of reaction must be sufficiently close to 0.65; the LAM order of reaction must be sufficiently close to 2.0. Note that the SRE rate constants used in CellSage have default units of inverse weeks if a time basis is used during regression. If a per-cycle basis is used then the rate constant values should reflect the cycles-per-week basis. If all these conditions are met, and the sum of squares error associated with a possible set of parameters is less than the previous least sum of squares value, then that solution is chosen as the new best fit. Mathematically, these restrictions are shown as Equation 3 through Equation 10.

$$M + N \leq 100 \quad (3)$$

$$a > c \quad (4)$$

$$b < d \quad (5)$$

$$0.325 < \frac{M}{N} < 3.0 \quad (6)$$

$$|a - 0.1| < 0.095 \quad (7)$$

$$|c - 0.005| < 0.03 \quad (8)$$

$$|b - 0.65| < 0.35 \quad (9)$$

$$|d - 2.0| < 1.7 \quad (10)$$

If a proposed solution meets these requirements, and the sum of squares error is less than the previous sum of squares error associated with the previous best solution, the new solution is taken as the best, and is used to generate a family of new solutions. This process is repeated until a solution meets a predisposed criterion. In this case, the sum of squares error of an acceptable solution had to be less than a specified value.

Figure 4 displays the fitting outcomes attained using the genetic algorithm for the identical dataset depicted in Figure 2. This specific curve fitting result was accomplished in under five seconds using a modern Windows PC with 16GB of ram and a 12th gen Intel i-7 processor, yet the overall curve-fitting duration with the genetic algorithm is contingent upon both the noise level and length of the baseline aging dataset.

We recognize the importance of also looking at the uncertainty error for each SRE parameter. It is possible to achieve high R^2 and low sum-of-squares predictive error while still having high uncertainty errors for particular parameters. A rough rule-of-thumb is to achieve uncertainty errors that are less than 10% of each regressed parameter value. By doing so, spurious SRE outcomes are avoided and a higher confidence of the fit is attained.

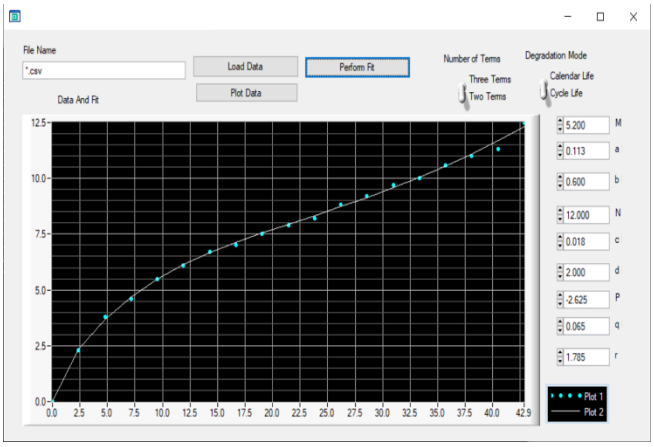

Figure 4: Dataset fit with genetic algorithm

Table 1 shows SRE parameter estimates provided from the following three sources:

1. Manual Non-linear least squares from third-party software
2. Automated Non-linear least squares from CellSage New Chemistry Import Feature:
3. Genetic Algorithm

Table 1. Initial SRE parameter estimates to compare.

	M	a	b	N	c	d
1	7.970	0.217	0.600	40.100	0.011	2.000
2	7.970	0.230	0.729	61.869	0.010	2.271
3	8.202	0.198	0.722	20.000	0.017	2.750

Inspection of Table 1 shows that the value of *N* determined with the genetic algorithm differs from the value of *N* determined using the non-linear least squares method by about 20 and 40 percent, and that use of the parameter values as inputs for the non-linear least squares fitting method are more consistent.

This result begs the question: what fitting method produces the most reasonable solution? This question would be best answered by long-term test data associated with the battery in question. However, such measurements are difficult to find. In the absence of such data, comparison of fitting results for a longer test time or larger number of cycles can offer some insight into which set of parameters might represent the better fit.

A comparison of result from evaluation of Equation 1 using each of the parameter sets from Table 1 is shown as Figure 5 and Figure 6. In each instance, the parameter sets resulted in curve fits with Mean Squared Error (MSE) below 0.02, indicating satisfactory performance in terms of curve fitting. However, there is observed variation in long-term behavior between the fits generated by the non-linear least squares method and the genetic algorithm. The left-hand plot of Figure 6 illustrates that while non-linear least squares fits suggest capacity loss progressing to approximately 65% to 70%, the genetic algorithm indicates asymptotic capacity loss nearing 30%. Despite this difference in long-term behavior, agreement in results persists until around week 75, representing roughly a 30-week extension beyond the data collection endpoint, as depicted in the right-hand side of Figure 4.

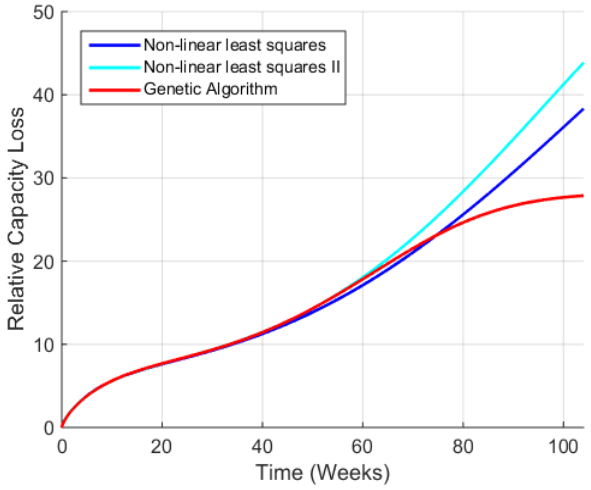

Figure 5: SRE results comparison up to 100 weeks.

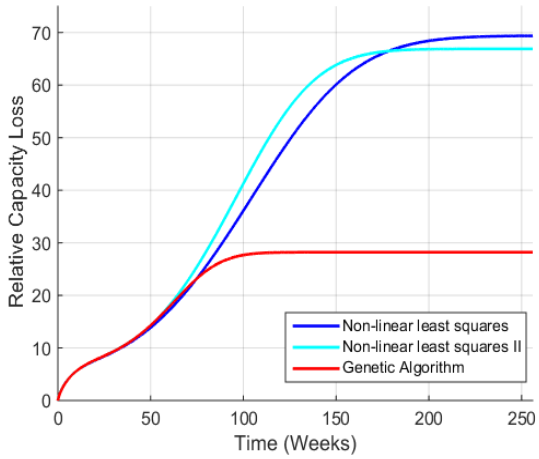

Figure 6: SRE results comparison up to 250 weeks.

Although these findings highlight certain limitations regarding the genetic algorithm's ability to produce SRE estimates with precise long-term outcomes, it excels in providing initial SRE estimates for the automated non-linear least squares method utilized in CellSage. Together, these capabilities have empowered Ridgetop, INL, and their collaborators to develop reasonable CellSage models with limited baseline aging data.

V. Model Comparison and Method Validation

To begin the model comparison and method validations we will review a of summary table for the calculated Sum of Squared Errors (SSE), Root Mean Square Error (RMSE), Mean Square Error (MSE), and R-Squared Coefficient (R^2) for each of the default cell chemistry models within CellSage. Each metric is calculated as follows:

- $SSE = \sum_{i=1}^{N}\left(y_i^{Data} - y_i^{Model}\right)^2$
- $MSE = \frac{SSE}{N}$
- $RMSE = \sqrt{MSE}$
- $R^2 = 1 - \frac{SSE}{SST}, SST = \sum_{i=1}^{N}(y_i^{Data} - y_{ave}^{Data})^2$

The following notes can be used to assess the quality of the fit based on each of the calculated metrics:

- SSE – The smaller the SSE, the better the fit.
- RMSE – The smaller the RMSE, the better the fit.
- MSE – The smaller the SSE, the better the fit.
- R^2 - The closer to 1.0, the better the fit.

In addition, checking parameter-wise uncertainty errors is highly recommended for each dataset under regression. Often, improvements in lowering such errors can be seen by providing better upfront estimates for the SRE parameters.

For the second set of model comparison exercises, Ridgetop and INL have prepared Figure 7 - Figure 14

to qualitatively assess the accuracy of using the SRE results from cycle life one, to model cycle life two temperature conditions. Note that the only difference between cycle life one and cycle life two is that cycle life two is associated with greater temperature than cycle life one. All other operating conditions are the same including the cell chemistry, form factor, and cycling rate.

Table 2. Summary Table of MSE, SSE, R^2, RMSE for Automated Non-linear least squares regression analysis of Cycle Life One data at lower baseline temperature.

	Chemistry Model	SSE	RMSE	MSE	R^2
1	LFP-graphite (A123 26650)	1.0097	0.3349	0.0673	0.9992
2	LFP-graphite (A123 Nanophosphate 20Ah)	0.2654	0.1429	0.0139	0.9986
3	LithiumCobaltOxide (18650)	0.3201	0.1051	0.009	0.9991
4	LMO-LTO (20 Ah)	0.0666	0.0354	0.0010	0.9969
5	NCA-graphite (DOE Gen2 18650-Model 1)	4.0927	0.3633	0.1106	0.9927
6	NCA-graphite (DOE Gen2 18650-Model 2)	3.0844	0.3154	0.0833	0.9909
7	NMC-graphite (Panasonic UR 18650)	6.6193	0.6643	0.3152	0.9946
8	NMC-graphite (Sanyo Y 18650)	0.7012	0.2162	0.0333	0.9976

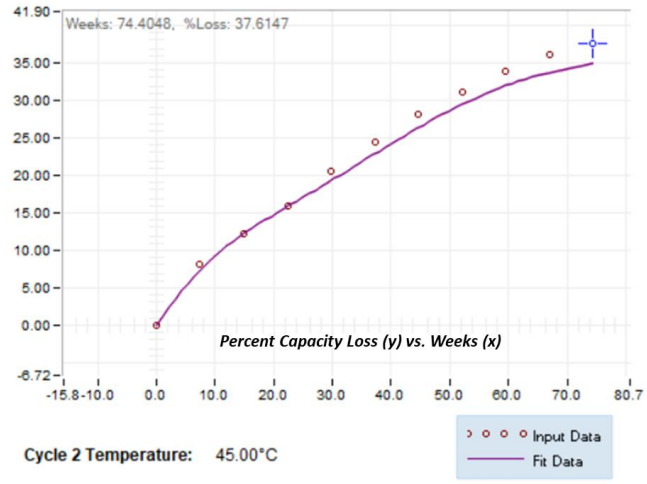

Figure 7: CellSage SRE Comparison for the LFP-Graphite (A123 26650) Battery Model.

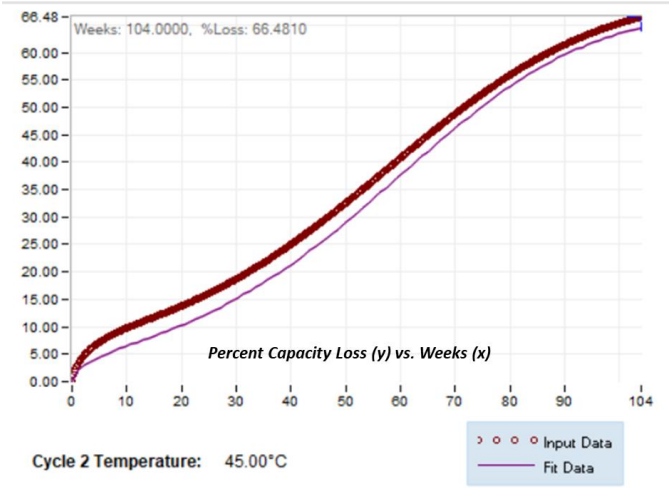

Figure 8: CellSage SRE Comparison for LFP-graphite (A123 Nanophosphate 20Ah) Battery Model.

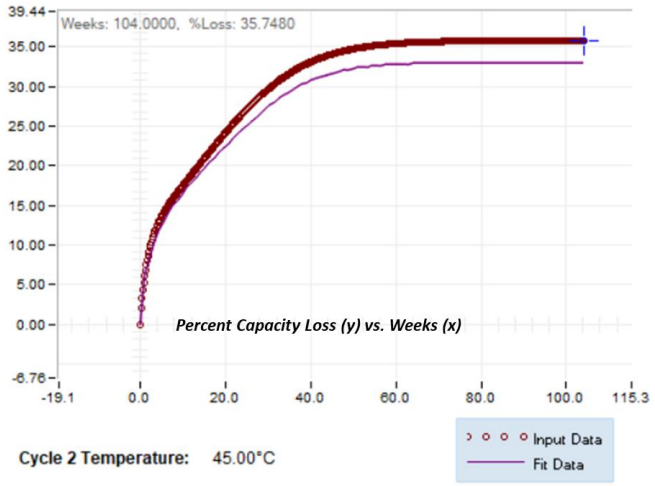

Figure 9: CellSage SRE Comparison for the Lithium Cobalt Oxide (18650) Battery Model.

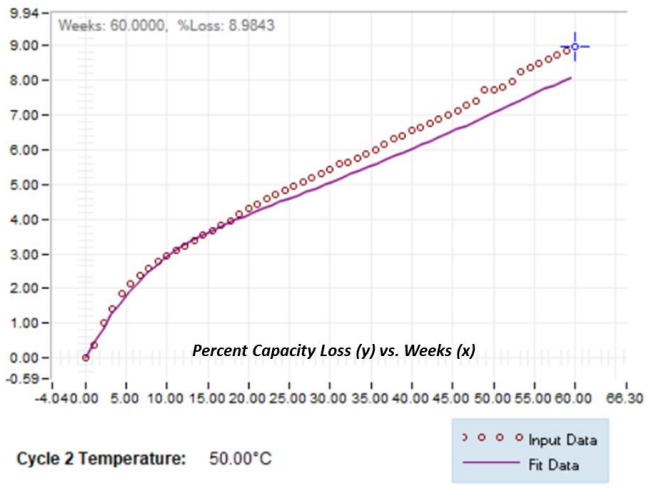

Figure 10: CellSage SRE Comparison for an LMO-LTO Battery model.

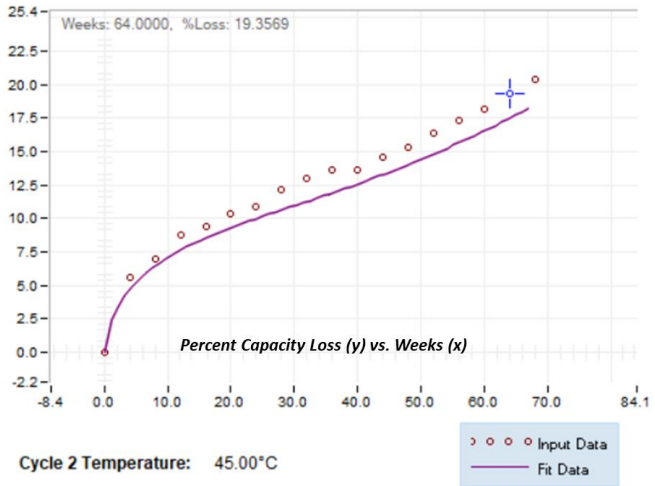

Figure 11: CellSage SRE Comparison for the NCA-graphite (DOE Gen2 18650- Model 1) Battery Model.

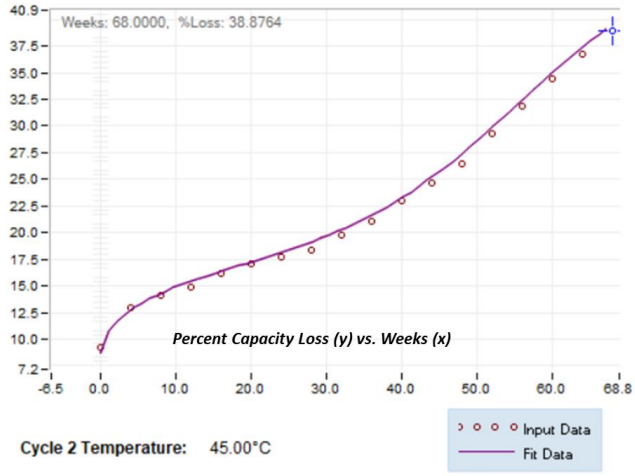

Figure 12: CellSage SRE Comparison for NCA-graphite (DOE Gen2 18650- Model 2) Battery Model.

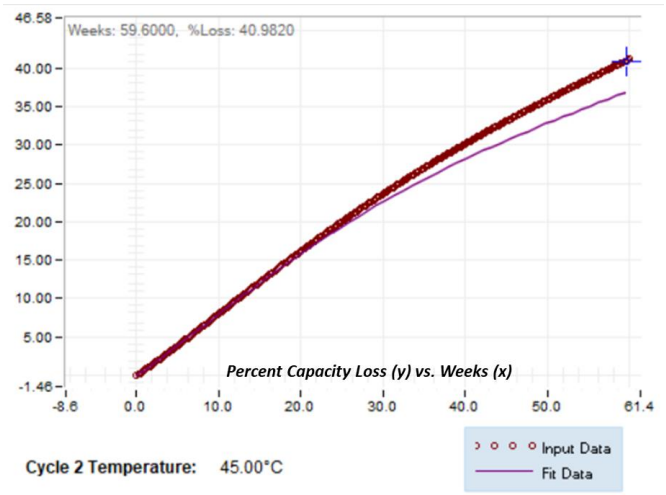

Figure 13: CellSage SRE Comparison for the NMC-graphite (Panasonic UR 18650) Battery Model.

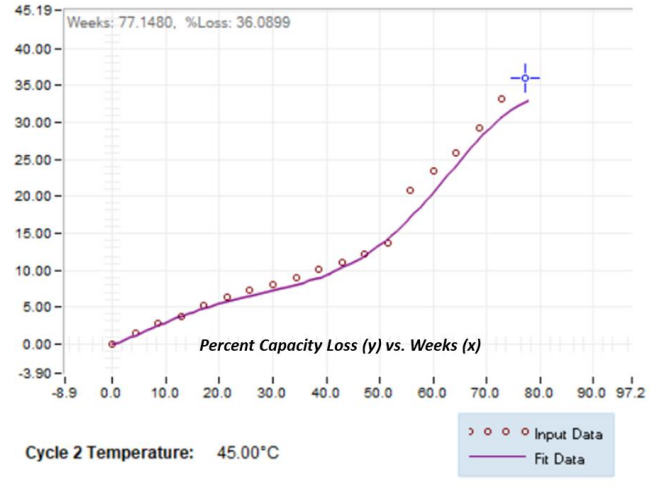

Figure 14: CellSage SRE Comparison for the NMC-graphite (Sanyo Y 18650) Battery Model

VI. Summary and Conclusion

Based on Table 2 and Figures 7-14, the CellSage SRE results from cycle life one demonstrate both quantitative and qualitative agreement when simulating baseline aging data at cycle life two, despite the latter being associated with a higher testing temperature. This observation highlights the robustness of the models and methods employed.

To validate the models, Table 2 was utilized to analyze metrics such as Sum of Squared Errors (SSE), Root Mean Square Error (RMSE), Mean Square Error (MSE), and R-Squared Coefficient (R^2) for each default cell chemistry model within CellSage. Lower SSE, RMSE, and MSE values indicate better fits, while R^2 values closer to 1.0 signify stronger fits.

Several chemistry models in Table 2 exhibit remarkably low error metrics, such as the and other models like the LMO-LTO model like the NMC-graphite (Panasonic UR 181650) model demonstrate slightly higher error metrics. Nonetheless, it's crucial to emphasize that all cell chemistry models adhere to the boundary conditions set by the underlying physics-based logic governing CellSage. One important takeaway is that accuracy and model fidelity typically increases with increased test cycles as the SREs can be calibrated to the maximum extent of the dominant aging mechanisms such as LLI and LAM. Additionally, it's essential to recognize that model fidelity can vary depending on factors such as cell chemistry, baseline testing equipment, sampling rate, size of aging dataset, and several other environmental operating conditions during the data acquisition process.

Qualitative assessment through Figures 7-14 confirms the accuracy of using SRE results from cycle life one to model cycle life two under different temperature conditions. Despite the increased temperature in cycle life two, the consistency in results underscores the reliability of the modeling approach, given that all other operating conditions remain constant, including cell chemistry, form factor, and cycling rate. These findings support the efficacy of the utilized methodology and contribute to the validation of CellSage models for predicting battery behavior under varying conditions.

In summary, this collaborative effort between Ridgetop Group and Idaho National Laboratory aimed to enhance the CellSage battery health modeling, simulation, and analysis software platform, enabling predictions for batteries with necessary baseline aging data. Automated regression analysis methods were developed to extract essential model parameters for SREs, enhancing the platform's efficacy in predicting battery aging under diverse operating conditions. Overall, these findings validate the enhanced CellSage platform as a valuable tool for battery manufacturers, researchers, and integrators worldwide.

VII. Acknowledgements

This research and development endeavor was made possible in part by the support of the U.S. Department of Energy (DOE) through a small business innovation research (SBIR) program, under award number DE-SC0023738. We express our gratitude to the DOE for their invaluable contribution to this project.

Additionally, we extend our sincere appreciation to Dr. Kevin Gering at Idaho National Laboratory (INL), whose expertise in electrochemistry and battery health modeling has been instrumental to the success of this endeavor. Dr. Gering's unwavering dedication and guidance have played a pivotal role in mentoring and fostering the growth of a world-class team at Ridgetop Group. We are profoundly grateful for his significant contributions to our research and development efforts.

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