Mission-Specific Prognosis of Li-ion Batteries using Hybrid Physics-Informed Neural Networks

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Abstract

New transportation modalities such as electric powered vertical takeoff and landing aircraft and logistic applications like delivery of packages with drones require highly reliable and powerful electric batteries for operation. A challenging but very important task hereby is the precise forecasting of the degradation of battery state-of-health (SOH) and state-of-charge (SOC). While high-fidelity electrochemistry based models can provide precise predictions of the SOC, they can be computationally expensive. On the other hand, purely data-driven approaches require a large amount of training data in order to learn the input to output relation. In this research an improved hybrid physics-informed machine learning model is introduced, that conserves the electrochemistry based laws and is implemented with data-driven layers to compensate for unknown portions of internal voltage drop during discharge. Preliminary results indicate that the model can predict discharge for a large variety of loads, accurately predicts capacity degradation over age and can be enhanced through extracting information from cell temperature data as surrogate for aging.

1. Problem Statement

State-of-the-art Li-ion battery cells are a crucial part of the electric powered vehicles and contribute up to 40% of vehicle cost (Lutsey & Nicholas, 2019). Hence, there is a demand in models that can predict SOH and SOC depending on wide load level variations taking into account the underlying electrochemistry of Li-ion battery cells. The existing modeling approaches that have been trying to address these challenging predictions have found the following roadblocks:

- Purely model based approaches have difficulties to replicate the complex non-linear behavior of battery aging processes without using experimental validation data.
- Data-driven approaches require a large amount of data that come along extensive efforts to build test beds for battery aging under real-world conditions.
- Time constraints associated with experimental testing of battery life make it impractical to gather data from real life operation for prognosis of battery health degradation.

In this PhD research we aim to address these roadblocks by (i) developing a physics-informed machine learning model, which uses previously gathered data on battery degradation and aims to forecast the SOH and SOC degradation on new developed battery cells with only some available data history; (ii) validating the trained model against gathered data from a accelerated battery life aging test conducted on a self-designed battery cycling test bed; and (iii) contribute to the state-of-the art literature regarding Li-ion battery degradation through implementation of a new model using additional available sensor data (e.g. cell temperature) for SOH prediction.

2. Contributions to the State-of-the Art

The main output of this research is a physics-informed machine learning model for battery degradation prognosis that:

- Estimate SOC during constant and variable current discharge depending on load levels
- Track and forecast capacity degradation over lifetime as function of operating conditions
- Predict Battery failure taking into account current levels and temperature build-up during discharge

The resulting hybrid physics-informed machine learning model is designed to accurately estimate remaining useful life of Li-ion batteries and detect battery cells that are close to failure and require replacement. The model is also designed to be deployable for different Li-ion battery cell chemistries by utilizing readily available data from fleet operators and minor adjustments of model parameters.

3. Research Plan

The specific objectives of this research include these four primary tasks:

Objective 1: Develop a test bed for accelerated lifing of Li-ion batteries- Design an accelerated battery lifecycle test bed that utilizes integrated self-designed printed circuit boards to autonomously cycle Li-ion battery cells. The goal is to gather a rich dataset of battery aging depending on load level variations as training data for hybrid machine learning models.

Objective 2: Implement an algorithm for solving ordinary differential equations using hybrid physics-informed neural networks- In this task we develop a new machine learning approach that implements hybrid models combining physics-informed and data-driven kernels, where data-driven kernels are used to reduce the gap between predictions and observations of time series forecasting.

Objective 3: Create a framework for pro-active monitoring of new components using Bayesian transfer learning- The goal here is to build a transfer learning model that uses a combined electrochemistry based and machine learning approach to predict SOC and SOH of Li-ion batteries taking into account battery fleets with large load level ranges.

Objective 4: Develop a method for battery degradation prognosis as function of cell temperature and load levels- Using temperature build-up and current data from discharge cycles we aim to build a Bayesian model for remaining useful life and failure prediction.

3.1 Progress to date

In the first step of this PhD research, we designed and built a test bed for accelerated battery life testing that integrates self-designed printed circuit boards, which, in combination with a microcontroller, perform continuous full charge and discharge cycles of battery packs at controlled current levels. Here, we contribute to the literature by generating a life cycle dataset for batteries subjected to a wide range of load levels with either constant or variable loading conditions. This rich dataset allows to study battery aging under real world operating conditions, as they are expected in battery powered vehicles. With the goal of building a hybrid battery degradation model, we estimate the battery capacity at each 20th cycle through reference discharges at constant current levels of 1C. Fig. 1 (left) shows the self-developed testbed in operation, where 6 battery packs placed on separate levels are connected to one charger board each and a load board, used for discharge, is placed on the top level. In Fig. 1 (right) the capacity degradation over cumulative energy, generated from our life cycle study, is shown for each battery until reaching end of life (marked by X). By collecting this dataset we already contribute to the literature for battery aging research, covering a wide battery aging range, which is used in this research as foundation for battery degradation prognosis with hybrid machine learning.

In the second part of this research, we implemented a Python framework for the solution of ordinary differential equations through recurrent neural networks (RNN) as further detailed in (Nascimento, Fricke, & Viana, 2020). This approach is used to build hybrid models, where ODEs governing reduced order

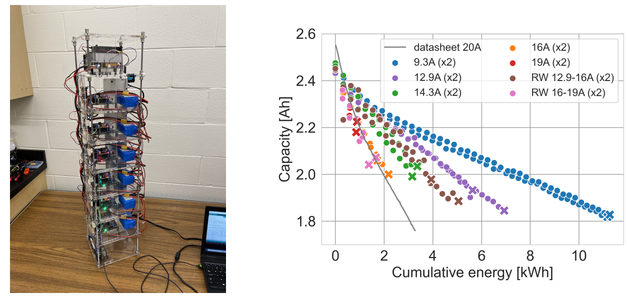

Figure 1. Testbed for battery lifing and capacity degradation.

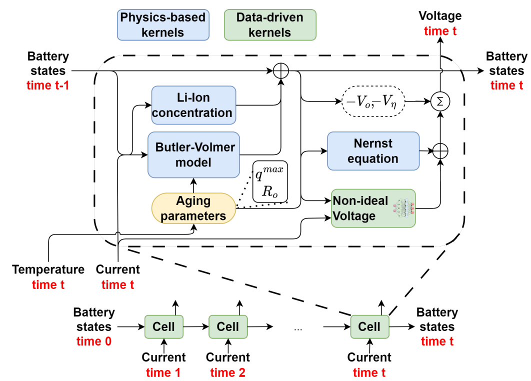

Figure 2. Hybrid physics-informed battery discharge model

physics equations are implemented in a recurrent neural network cell and a machine learning compensator is used to learn the missing physics of the reduced order model. To demonstrate the capabilities of this approach, in one case study we implement fatigue crack growth integration through Euler's forward method combining a data-driven stress intensity range model with a physics-based crack length increment model in order to reduce the gap between predictions and observations. In a second case study, we implemented a two degree of freedom mass-spring-damper system within an RNN cell, where parameter identification of the damping coefficients could be successfully demonstrated.

Using this RNN integration framework we extend the capabilities of the RNN cell by implementing a hybrid electrochemistry and data-driven battery SOC model to predict the voltage curves during discharge depending on current and battery cell temperature inputs (Fig. 2). The cell predicts the voltage output at each time step, where the state, similar to a state space representation, is integrated over the entire time series. The general voltage drop is captured through the Nernst and Butler-Volmer equations (blue blocks), as introduced in (Karthikeyan, Sikha, & White, 2008) and (Daigle & Kulkarni, 2013), while the remaining discrepancy between actual and predicted voltage is captured through the non-ideal voltage multi-layer perceptron (green block), as it was presented by (Nascimento, Corbetta, Kulkarni, & Viana, 2021).

Our contribution here, further enhances the hybrid approach by introducing the effects of large load variations and cell temperature build-up during discharge to the prediction model. The proposed model is trained, on constant loading discharge curves detailed in Fig. 3, whereas the variable loading curves are used for validation. Fig. 4 illustrates the discharge prediction results on early life variable loading (top) and predictions on the same battery later in life (bottom), where our findings validate that the model predictions significantly improve through aging parameter updates. The aging parameters in form of available Li-ions (q^{max}) and internal resistance (R_b) are updated using battery discharge curves throughout cycle life. Fig. 5 shows our Gaussian process model (GP) predicting the degradation of q^{max} and the increase of the internal resistance R_b as function of cumulative energy and loading levels, where our model captures the influence of different load levels on both aging parameters.

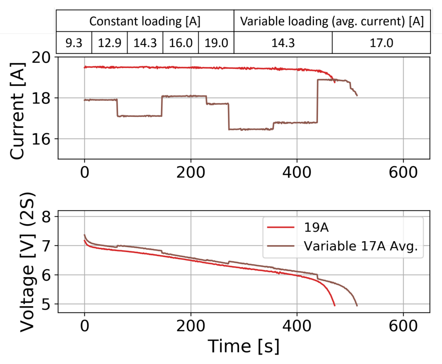

Figure 3. Current and voltage discharge curves

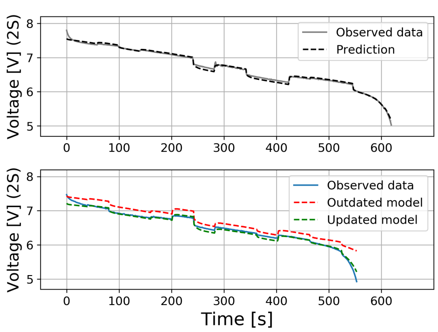

Figure 4. Random loading discharge prediction on early life (top plot) and aged battery (bottom plot) with updated and outdated model parameters

Fig. 6 shows the cross validation results for a prediction outside of the training dataset, where the lowest load level at 9.3A was partially or completely excluded from training data and used for prediction. Our findings indicate, that without any early life data (left column) predictions for q^{max} and R_b deviate from the data points, whereas updating the model with early life data until 6kWh (right column) significantly improves the prediction results.

Using the predicted aging parameters we established predictions of discharge curves on aged batteries. Fig. 7 shows the discharge curve prediction for 9.3A load level at a battery age of 4kWh and 6kWh, respectively. Without early life data, the model prediction deviates from the discharge curve, whereas our investigation shows, adding early life data helps to improve the discharge curve prediction significantly.

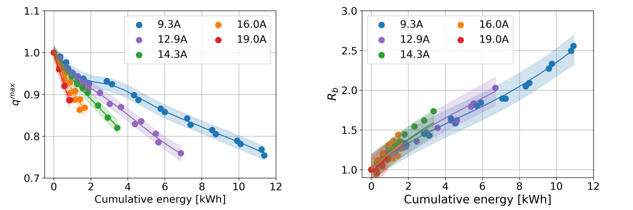

Figure 5. Gaussian process model for q^{max} and R_b over lifetime with mean function and 95% CI.

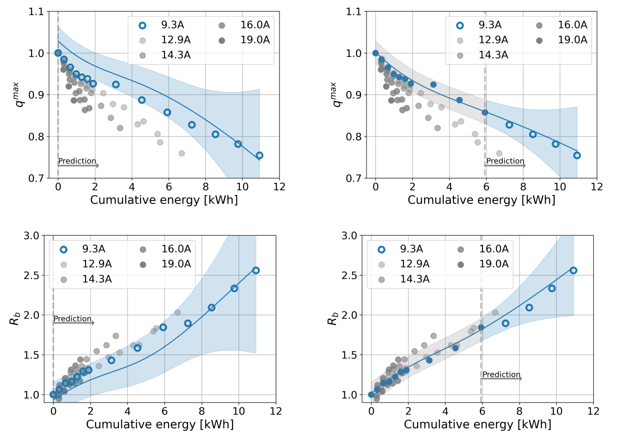

Figure 6. Forecast of q^{max} and R_o as function of cumulative energy for constant current at 9.3A. Predictions are done with and without q^{max} and R_b update using early life data.

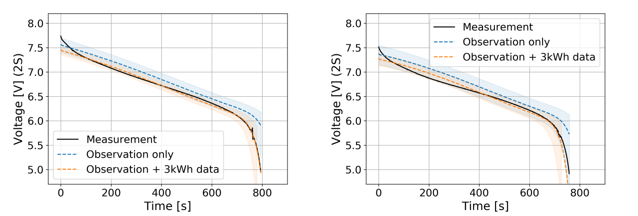

Figure 7. Voltage curves for 9.3A constant discharge at 4kWh (left) and 6kWh (right) using predicted q^{max} and R_b.

3.2 Remaining work

We will further contribute by enhancing the model to predict cell failure and using temperature build-up data during discharge cycles as surrogate for age. Fig. 8 shows the failure classification including 95% confidence intervals (CI) for different load levels as function of cumulative energy. The presented GP model already establishes a prediction method for battery failure as function of age on different load levels and will be fused with the battery aging model in the next step.

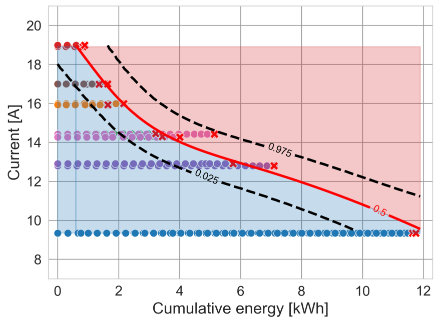

Figure 8. Failure classification: current levels vs age

Furthermore, we propose a model using cell temperature build-up during discharge cycles to predict aging curves and failures. In Fig. 9 one can see a clear trend between the within-mission temperature build-up and battery age (Fig. 9, left). Here, we will contribute by extracting the slope of the temperature curves to build a GP capacity prediction model with load level and temperature slope as input (Fig. 9, right).

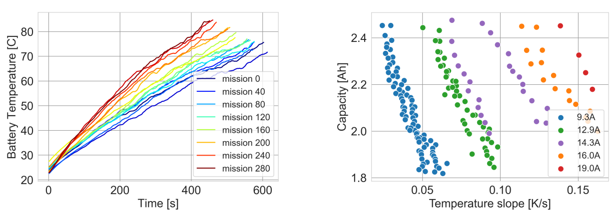

Figure 9. Capacity as function of cell temperature.

In this research we also propose a model to capture loading variations over life time. Fig. 10 shows the capacity degradation curve (full circles) of a battery that was initially aged at 16A until reaching 2.15Ah, moved to a mild load of 7.5A until 2.0Ah and aged at a more aggressive load of 17.5A until failure at 1.92Ah. Here, we will establish a model that can predict battery degradation depending on load level changes, where the model is used to move the battery to an equivalent age at the current load level (empty circles). Additionally, we contribute through re-using previously aged battery cells. For this purpose, previously deployed cells with similar aging history were assembled to new battery packs. Those second life battery packs are then subjected to milder load levels compared to the initial deployment. Fig. 11 shows the capacity degradation curves of four second life batteries, where significant life extension of up to 4kWh has been observed. With this approach we will introduce a model that can be beneficial for operators of battery fleets that intend to re-purpose used battery cells.

4. Conclusion

In this research work an enhanced hybrid physics-informed machine learning model is proposed to predict the SOH and SOC of Li-ion batteries. Through a self-designed test bed

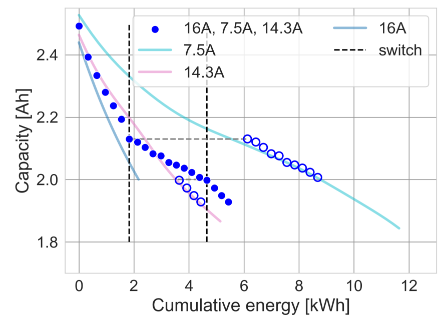

Figure 10. Battery recommissioning from aggressive (16A), to mild (7.5A) and moderate loading (14.3A).

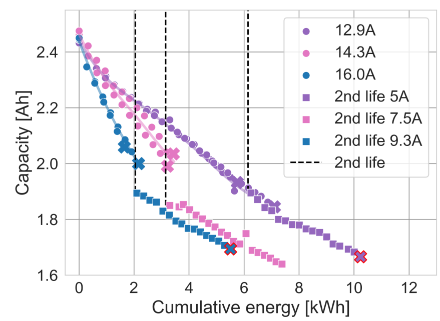

Figure 11. Aged batteries with 2nd life at low current levels.

battery life cycle data gathered and used to train a hybrid electrochemistry based and data-driven model in order to capture missing physics for discharge voltage prediction. Preliminary results show the model can predict variable and constant load discharge curves and can successfully predict the the aging parameters to determine SOH as function of loading conditions.

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