Battery safety: Data-driven prediction of failure

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Abstract

Accurate prediction of battery failure, both online and offline, facilitates design of safer battery systems through informed-engineering and on-line adaption to unfavorable scenarios. With the wide range of batteries available and frequently evolving pack designs, accurate prediction of cell behavior under different conditions is very challenging and extremely time consuming. In this issue of Joule, Li et al. used data from a previously reported finite-element model to train machine learning algorithms to predict whether a cell will undergo an internal short circuit when exposed to a selection of mechanical abuse conditions. The presented approach aims to alleviate, and yet is still limited by, a common challenge facing data-driven prediction methods; access to robust, plentiful, high-quality and relevant experimental data.

Lithium-ion batteries are now ubiquitous in society, with wide-ranging applications from toothbrushes to satellites. The principal motivation for the recent exponential increase in battery production is to equip electric vehicles, which are quickly populating cities and towns around the world. In electric vehicles and for other demanding applications, a high level of safety for lithium-ion battery systems is critical. The spectrum of conditions that can lead to failure of a cell, as well as the consequent failure mechanisms and risks, is vast. With continuously evolving cell and battery designs, understanding the causes and consequences of the entire spectrum of failure scenarios through laboratory tests is not feasible. Computational modelling can be used to reduce the number of experiments required to map this space, but even this approach can be limited by computation power and robust validation. Researchers from Ford Motor Company have recognized this, and have recently made a call for a more elegant means of determining the response of continually evolving cell designs to different hazardous conditions to be developed[1].

The application of data-driven techniques for identifying materials[2] and predicting the lifetime and performance of Li-ion batteries[3] has shown promising results and has ignited interest in exploring data-driven methods in improving predictive capabilities for cell behaviors[4]. Progress in the collection and processing of big-data have opened the possibility of on-line learning and prediction of battery behaviors. For example, using voltage and capacity data from the first 100 cycles (ca. 10% of their total life) of 124 commercial cells of the same type, Severson et al.[3] trained a simple regression model that could predict the cycle life with ca. 90% accuracy. But how can data-driven techniques be applied to prediction of catastrophic failure of Li-ion batteries? And can they provide an elegant solution to understanding and efficiently predicting the response of next generation cell and pack architectures to real world conditions,

in order to improve the safety of battery systems?

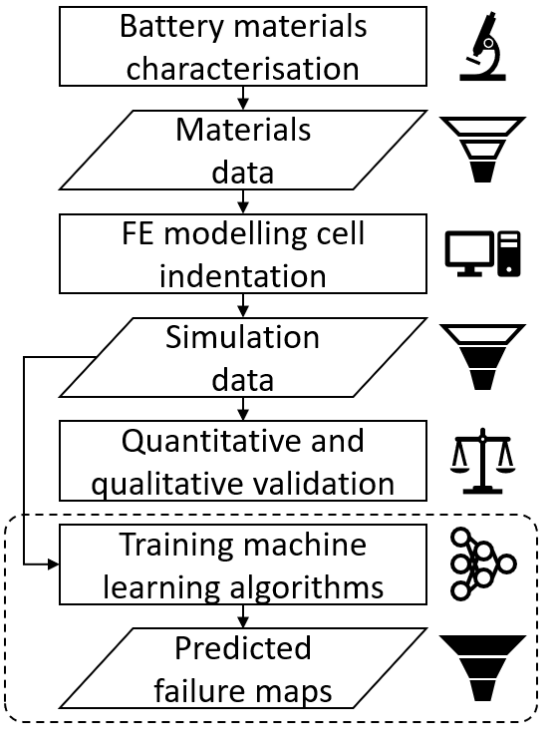


Figure 1. Flow diagram showing the layered structure of the approach by Li et al.[5]. The first section is described by Zhu et al.[6] and the dashed box shows the work described by Li et al.[5]. The icons give an indication of either the nature of the activity or the size of the dataset created at this stage.

In a recent publication by a team from the Massachusetts Institute of Technology and Tsinghua University, Li *et al.*[5] presented an approach to mapping the risk profile of a range of impact scenarios, whilst trying to minimize both the experimental burden and the computational cost of detailed modelling. The team leveraged a finite element (FE) model[6] based on data from systematic materials testing and the selection of materials specific deformation mechanisms. The model showed good quantitative agreement with quasi-static strain experiments (although, as the authors note, data from dynamic tests would be more relevant to this application), as well as reasonable qualitative agreement with failure modes observed using tomographic imaging. A significant data pool was generated using this model, exploring a wide variety of different mechanical abuse conditions (shape, speed and angle of attack of the indenter), which was in turn used as the training data for the following two supervised machine learning (ML) models: a classifier, which was trained by defining failure as the moment when the separator breaks within the FE models; and a regression model, which evaluated the deformation characteristics necessary to cause breakage. This led to the construction of a data-driven "safety envelope", or range of safe operating conditions of cells.

The prospect of carrying out a minimal experimental package to predict the behavior of cells across a wide variety of impact scenarios is very appealing, but the results should be interpreted with caution. The supervised ML approaches used in this study are trained entirely on the results of the FE simulations and can smoothly interpolate between them, but not extrapolate beyond them. The accuracy of the ML models depends on the accuracy and validity of the simulation, which in turn depends on the quality of the experimental data; a degree of separation exists between the ML model and experimental data as is clear from Figure 1. Ultimately, when modelling complicated objects, high quality experimental data is a necessity. However, an interesting advantage of Li *et al*'s approach is that, in principal, minor modifications in cell design (such as changes in the number of layers or the thickness of layers) can be incorporated into the FE model and the ML representation can be in-expensively updated. However, in order to trust a safety critical model, a full experimental validation would likely still be required; particularly as mechanical properties can vary greatly with conditions such as

temperature and electrolyte wetting, a limitation that the authors mention. Changes in temperature, cell packaging, and even variations in particle morphology may also have a significant effect on the observed behavior. Even the most cutting-edge manufacturing techniques suffer from batch-to-batch and cell-to-cell variance, as Severson et al.[3] observed when 124 cells of the same type degraded electrochemically at very different rates. Both the trained ML model and its FE based training data were fully deterministic and so cannot capture this variance, which in turn makes it difficult to assign a confidence value to the results for any particular cell. Furthermore, automotive pouch cells are universally contained with a protective casing, which makes the translation of cell-only predictions into real-world safety even more complex.

The probability of a cell to catastrophically fail electrochemically is likely linked to historical exposure conditions such as voltage windows, operating rates, mechanical shock, and temperature, as well as potentially unmeasurable manufacturing defects. Such highly non-linear systems prompt interest in applying ML techniques as they are flexible and do not necessarily require any physical insight into the dominant failure modes. However, the challenge that researchers face is in acquiring training data, in particular of rare events. Big datasets from field scenarios involving catastrophic failure would improve the accuracy of data-driven models and perhaps eventually enable predictions of the likelihood of catastrophic electrochemical failure, based on slight deviations in cell behavior. In order to be robust, data-driven methods require data from large experimental matrices covering a wide range of conditions, where multiple factors linked to battery health and safety would be measured. Some groups have published datasets of battery failure consisting of hundreds of cells, such as from NASA[7], NREL[8] and Tsinghua University[9], but none of the experiments were optimized for training classifiers, and the datasets are likely far smaller than what would be required to capture the expansive volume of failure scenarios, cell responses, and risks.

How then to get relevant data? Some of the major electric vehicle manufactures monitor their vehicle's battery systems out on the field and store the data; however, these extensive datasets are not made readily available to the academic community. Battery failure is extremely rare, so gathering statistically significant information on the lead up to failure would require, perhaps, cycling hundreds of millions of commercial cells of the same type. To put this into perspective, as of October 2019 Tesla have sold around 750,000 vehicles containing 4000 to 8000 cells each, totaling over 4 billion cells out on the field, whilst the total number of battery fires have been in the tens. Just as social media companies like Facebook provide veiled data to sociology researches for analyzing human responses, it would be beneficial for researchers to have access to the data that electric vehicle manufacturers have on vehicles out on the field.

Until access to larger datasets is achieved, innovative methods for optimizing experimental conditions, and perhaps broadening datasets through additional FE modelling is needed. For example, the FE step of the coupled FE and ML method described by Li et al., could be applied for cell types and conditions under which actual field failures occurred, and then be used with relative computational efficiency to interpolate between the conditions and provide a broader understanding of the cell's response. In particular, this technique could facilitate identification of risk-zones that account for the history of a cell and its present operating conditions. Accurate online predictive capabilities in battery management systems could present a breakthrough in battery safety. Accurate prediction could alleviate the hazard by avoiding failure completely through removing,

isolating, or replacing cells that pass into the predicted risk-zone, without sacrificing system performance that often accompanies alternative safe materials and safety devices.

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