Big data for lithium-ion battery diagnosis and prognosis

Matthieu Dubarry & David Beck
HNEI Hawai'i Natural Energy Institute
School of Ocean and Earth Science and Technology
University of Hawai'i at Mānoa
matthieu@hawaii.edu

Introduction

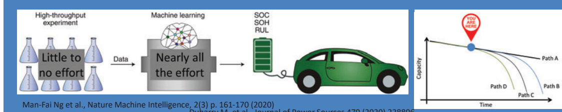
Accurate lithium-ion battery diagnosis and prognosis **is critical to increase penetration of electric vehicles and grid-tied storage systems**.
Diagnosis and Prognosis are complex tasks due to the **intricate, nonlinear, and path-dependent** nature of battery degradation.

The development of Data driven methods for Li-ion battery diagnosis and prognosis is a growing field of research for the battery community.
A big limitation is usually **the sizes of the training datasets which are typically not fully representative of the real usage of the cells**.

The aim of this work to provide the battery diagnosis and prognosis AI community with **comprehensive synthetic data sets** that can be used for statistical or deep learning methods.
This work also provides a detailed statistical analysis of the datasets. Accurate diagnosis as well as early prognosis were demonstrated using the combined information of three learnable parameters.

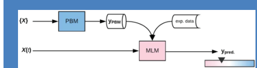
Objective & Significance

Gathering experimental data is extremely costly and time consuming. As a result, most studies only test **a small number of batteries to validate their algorithms**. This is vastly insufficient because Lithium ion battery degradation is **path-dependent** and small changes in conditions were shown to lead to drastic differences in durability. This path dependence is an **essential aspect to consider for the validation of diagnosis and prognosis tools**. With a limited set of training data, the universality of the tool cannot be validated.



Man-Fai Ng et al., Nature Machine Intelligence, 2(3) p. 161-170 (2020)
Dubarry M. et al., Journal of Power Sources 479 (2020) 228806

Online databases, like *battery archive*, and initiatives like *battery data genome* are steps in the right direction, but **state of the art is far from the big data needed to make AI work.**

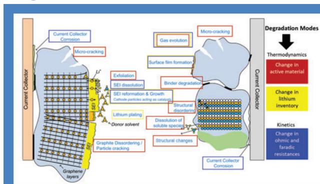


Aylol et al., Journal of The Electrochemical Society, 2021 168 030525

A possible solution is **transfer learning** to supplement experimental data with **synthetic data englobing the entire degradation spectrum**.

Generating such a variety of duty cycles will require a modeling approach that is **not calculation intensive and easy to parameterize**. Forward looking models, like traditional physics based models, might not be adapted because they require to parameterize equations for a wide variety of degradations. The backward looking **mechanistic approach** might be more adapted because it relies on emulating degradation modes.

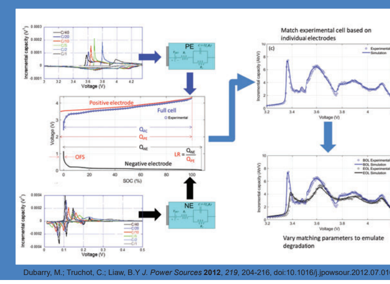
Degradation modes and Mechanistic Modeling Approach



Degradation modes refer to the **impact** of a mechanism rather than its root cause. Every degradation mechanism will impact the amount of material able to react, the amount of lithium able to go back and forth between the electrodes, and/or the overall reaction kinetics.
As such, three main families of degradation modes can be defined: **loss of active material (LAM), loss of lithium inventory (LLI), and kinetics changes**.
LAMs and kinetic limitations must be decomposed further at the electrode or electrode component levels for blends. Kinetic limitations must also address polarization and transport separately.

Full cell emulation is based on **half cell data** for each electrode (or each component of a blend) **at different rates.**
It only requires a **few parameters**:
- The **loading ratio (LR)**, the electrodes capacity ratio,
- The **offset (OFS)** that corresponds to the electrode slippage,
- The **rate** for each electrode (or component of the blend),
- The **resistance** for each electrode (or component of the blend).

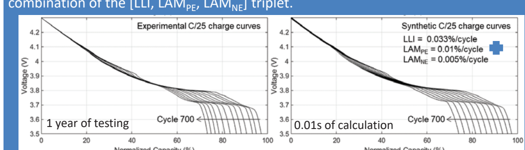
LAMs are emulated by changing the size of one electrode compared the other one and by adjusting the rate.
LLI is emulated by increasing the offset. This is because LLI is increasing the slippage between the electrodes.
Plating is emulated by considering the NE as a blended electrode
Plating irreversibility is simulated by increasing LLI



Dubarry, M.; Truchot, C.; Liaw, B.Y J. *Power Sources* **2012**, *219*, 204-216, doi:10.1016/j.jpowsour.2012.07.016

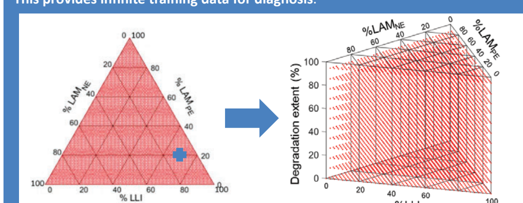
Building Synthetic Voltage vs. Capacity Datasets

From the mechanistic approach point of view, each thermodynamic degradation can be described by a unique combination of the [LLI, LAM_{PE}, LAM_{NE}] triplet.



It has to be noted that investigating blends and higher rates where kinetics and resistance needs to be considered will add parameters. ***This work only discuss thermodynamic degradations.***

The [LLI, LAMPE, LAMNE] triplets can be normalized so that their sum is equal to one and then can be represented in a ternary diagram. Scanning **every possible combination** of the triplet for **all degradation extent** yields any potential degradation from which the voltage response can be reconstructed.
This provides infinite training data for diagnosis.



Dubarry M. et al., Journal of Power Sources 479 (2020) 228806, Dubarry, M., et al. (2017)., Journal of Power Sources **360**: 59-69.

Published datasets:
>5,000 [LLI,LAM_{PE},LAM_{NE}] Combinations with at least 0.85% resolution.
This equates to 700,000 V vs. Q curves each for LFP, NCA, NMC811 vs. graphite

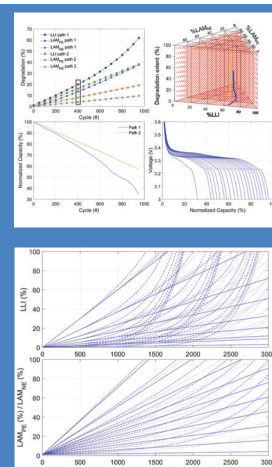
Mendeley Data, 2020; Vol. 2021, 10.17632/6s6ph9n8zg.3
Mendeley Data, 2020; Vol. 2021, 10.17632/bs2j56pn7y.3
Mendeley Data, 2021, 10.17632/2h8cpszy26.1
Mendeley Data, 2021, 10.17632/pb5xpv8z5r.1

Building Synthetic Duty Cycles Datasets

In this work, a duty cycle is defined as a **unique evolution of the triplet values** (and of other parameters if blends or kinetics are involved). This allows to **simulate duty cycles without the knowledge of what conditions could have lead to such degradation** (rate, DOD, cutoffs, temperature…).

The triplet values could be calculated, per example, for different linear degradation paces, with paces linear combined with exponential variations, or with a delayed exponential increase, more representative of the real degradation of commercial cells.

Since the voltages associated with all the triplet values were **already calculated for diagnosis**, no additional simulations are actually necessary as the different degradation paths were all already calculated. They can **be reconstructed by following the evolution of the triplet values in the ternary design space** and the corresponding voltage and capacity variations can be accessed.

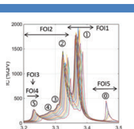


Published datasets:
>125,000 unique LLI/LAM evolutions with at most 1 curve every 100 cycles (> 3,000,000 V vs. Q curves total).
8 parameters varied following the **%deg = a ×cycle+ e$^{(b\times cycle)-1)}$** equation for LLI, LAM_{NE}, & LAM_{PE} plus a delay for the exponential for LLI (to simulate random knees) and 3 different plating reversibility (0, 50, 100%).

Using the Datasets: Diagnosis

Tracking **features of interest (FOI)** is a proven method to reach diagnosis. However, when tested over entire dataset, a **single FOI is never enough to get a good diagnosis.**
Considering the variations of **3 FOIs together** provides better accuracy.

Dubarry, M., et al. (2017)., Journal of Power Sources **360**: 59-69.



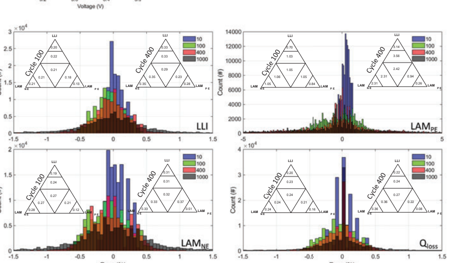
Correlation coefficients

	LLI	LAM_{PE}	LAM_{NE}	Capacity loss
FOI1	-0.74	-0.03	0.62	-0.72
FOI2	-0.03	0.09	-0.99	-0.06
FOI3	0.04	-0.36	0.73	0.07
FOI4	0.38	-0.17	-0.79	0.36
FOI5	-0.51	-0.26	0.78	-0.47
FOIs(1,2,3)	0.99	0.44	0.98	0.99
FOIs(1,2,4)	0.99	0.80	0.99	0.99
FOIs(1,2,5)	0.99	-0.07	0.98	0.99

For the >125,000 LFP duty cycles, the **mean diagnosis error was always below 0.8%** when using FOIs 1,2, & 4 together.
Independent study showed that our FOI based method **is more accurate than data-driven ones**.

Mayilvahanan, K., et al. (2021), Batteries & Supercaps 2021, 10.1002/batt.202100166

The insets presents the standard deviations at cycles 100 and 400. This reveals the **impact of the degradation mix on the accuracy of the approach.**



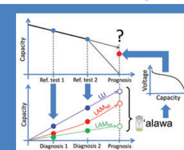
Beck. D., et al.Energies 2021, 14, 2371.

Using the Datasets: Prognosis

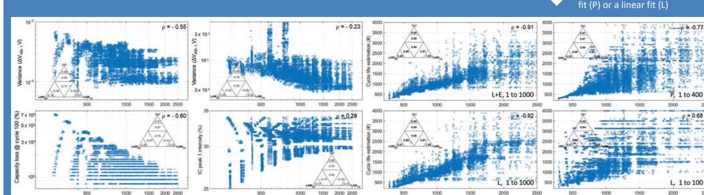
Many methods have been proposed in the literature for early prognosis.
The variance between cycle 1 and 100, the overall capacity loss and FOI1 for LFP are among the most used for a single point prognosis.

Correlations lower than reported where observed when tested on full datasets. Insets show that the correlation is **better on some subsets** (e.g. 0.9 for high LLIs for variance). This showcase the importance of testing on a varied dataset.

Prognosis established from diagnosis at different cycles shows better results with **much higher correlation coefficients**. They were established by fitting the evolution of LLI and LAMs using different cycle ranges and functions.



Prognosis using diagnosis at cycles 1 to X using a linear + exponential fit (L+E), a power fit (P) or a linear fit (L)



Conclusions & Perspective

- ✓ Proof-of-concept methodology to **generate big data training datasets,**
- ✓ Methodology could be **applied to different conditions such as rate and temperature,**
- ✓ Can handle **lithium plating with adjustable reversibility,**
- ✓ Ideal to **test validity of different approaches** for diagnosis or prognosis,
- ✓ Accurate data based diagnosis & prognosis were proposed **without needing AI algorithms**.

<u>This approach does not remove the need for experimental testing; it is still essential, and the only way, to decipher which conditions cater to specific degradation.</u>

Acknowledgments

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University of Hawai'i Mānoa
School of Ocean and Earth Science and Technology
HNEI Hawai'i Natural Energy Institute
School of Ocean and Earth Science and Technology
University of Hawai'i at Mānoa
-PakaLi+ Battery Laboratory