INL/CON-21-62775-Revision-0

Bat492: Machine Learning for Accelerated Life Prediction and Cell Design 2021

June 2021

Changing the World's Energy Future

Eric J Dufek

Idaho National Laboratory

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June 21-25, 2021

NREL
NATIONAL RENEWABLE ENERGY LABORATORY

INL-CON-21-62775

INL Idaho National Laboratory

Overview

Timeline

- Start: October 1, 2020
- End: September 30, 2022
- Percent Complete: 35%

Budget

- Funding for FY21 – $1.2M

Barriers

- Time needed to predict life and understand failure modes
- Lack of tools and methods which readily cascade across programs
- Distinct need to link physics to enhance the technology development process

Partners

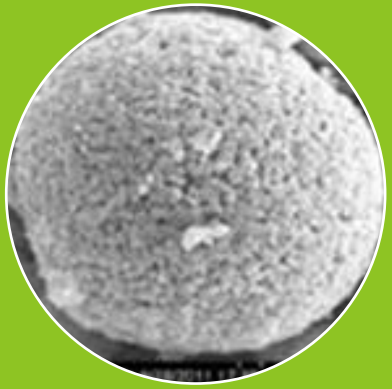
- Idaho National Laboratory
- National Renewable Energy Laboratory
- Close collaboration with Behind-the-meter-storage (bat442), and Extreme Fast Charge and Cell Evaluation of Lithium-ion Batteries (XCEL, bat 456-463 project)

Relevance

Objective: Accelerate transformative advancement by creating a robust, common framework

Develop methods and core tools to:

- Reduced time to validate new materials, designs, manufacturing processes and use cases
- Access to large amounts of data to enable discovery and deployment
- Provide breadth spanning transportation and stationary storage to support electrified mobility
- Benefit across the storage ecosystem (research to industry and consumers)



Materials Development, Understanding, and Manufacturing

Cell design, Validation and Manufacturing

System Integration and Deployment

Common Tools and Data Storage

Task milestones

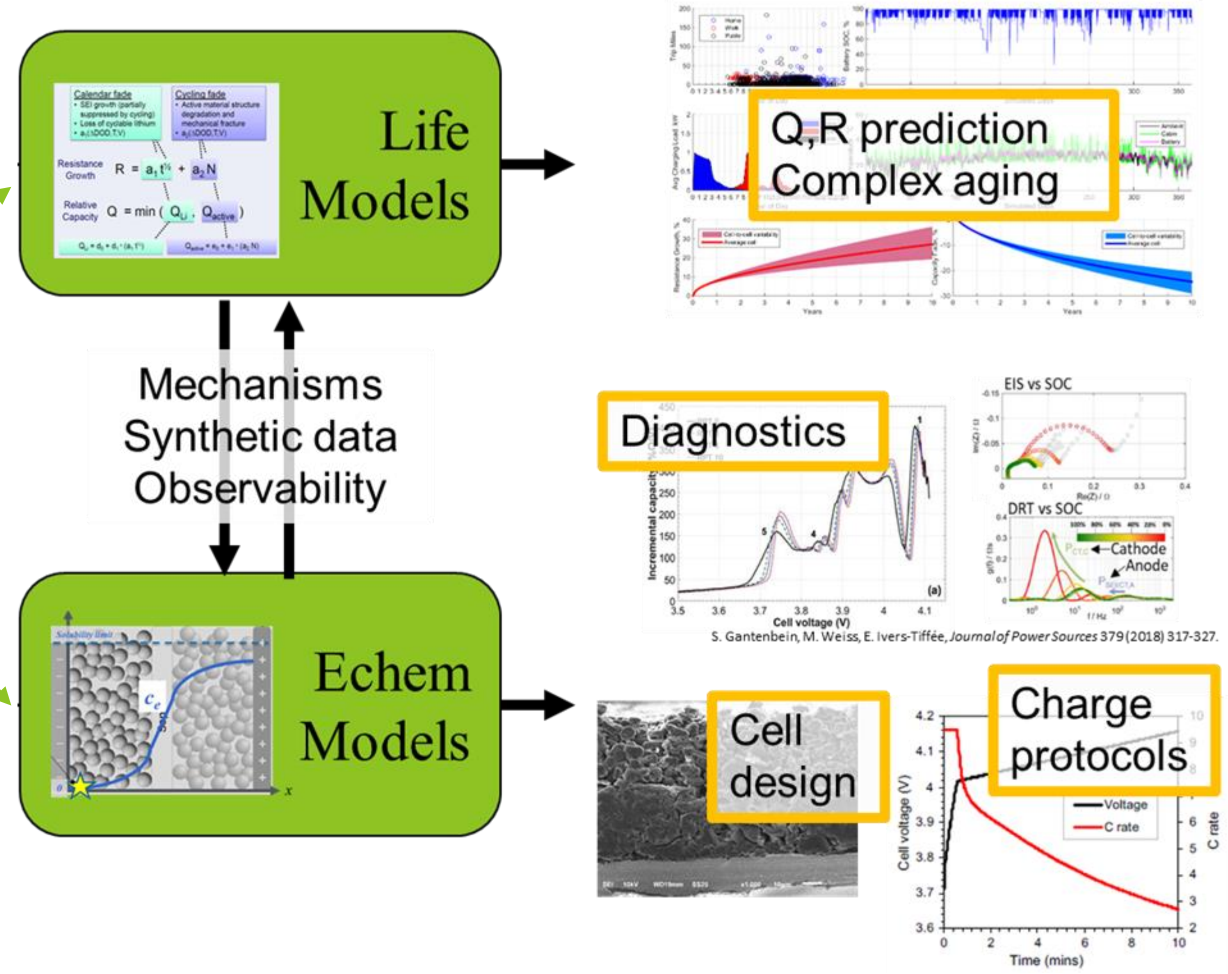
Milestone	Due	Status
Finalize IP structure and coordination across the team	12/31/20	Complete
Generate synthetic data from Graphite/NMC cells and initiate Deep Learning related to electrochemical signatures	3/31/21	Complete
Predict and validate electrochemical performance of aged cells for at least two different charging conditions using a combination of electrochemical and life models	6/30/21	In process
Quantify life model accuracy using automated physics-based model generation based on design and experiment duration using either LTO/LMO or graphite/NMC datasets	9/30/21	In process
Predict and validate performance and degradation modes within 5% for known duty cycles and 10% for use cases not aligned with training sets	9/30/21	In process

Approach

Accelerating innovation requires failure mode classification, projection and validation

Combination of high-quality data generation, assessment and analysis

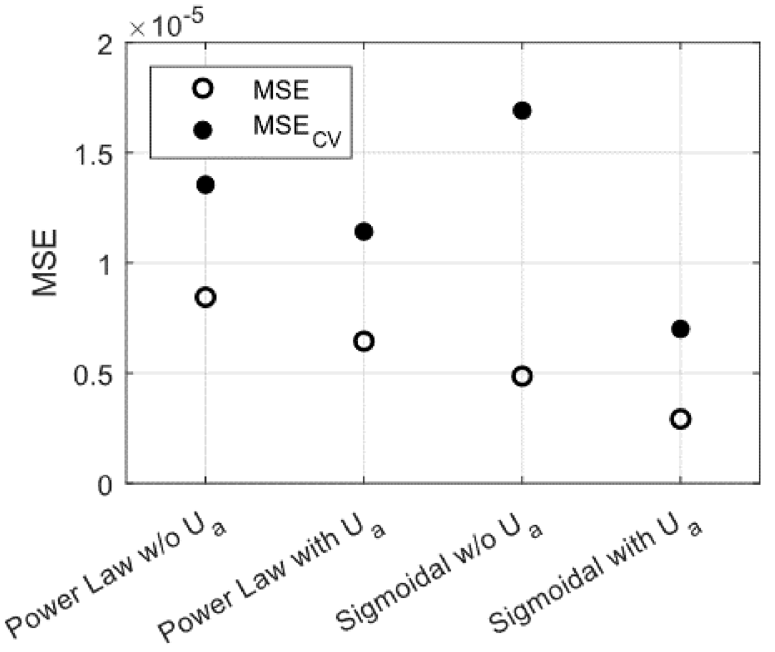
Use of robust electrochemical analysis with targeted secondary characterization for validation



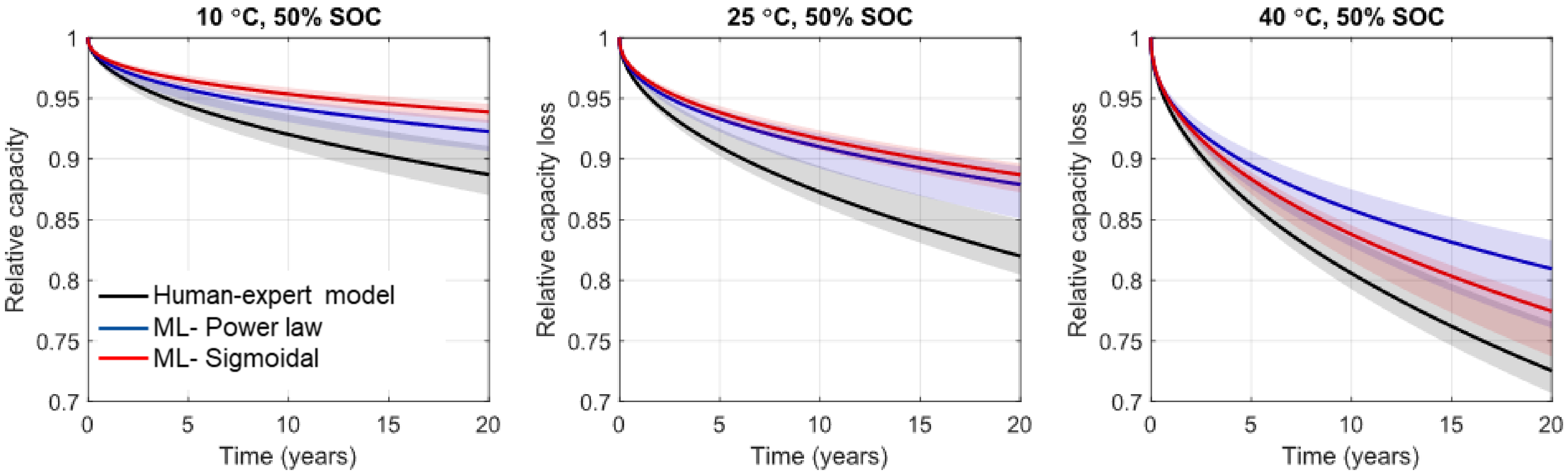
Early Understanding of Failure Modes to Reduce Development and Deployment Cost

Generation of algebraic battery life models

- Automatic identification of reduced-order degradation models
  - Bi-level optimization
  - Symbolic regression
  - Cross validation (CV)
- Up to 2x decreased uncertainty using autogenerated models when compared to human model development
- Methods include ability to perform sensitivity analysis and uncertainty quantification



Mean-squared error for auto-generated models



Calendar-life projections w/uncertainty

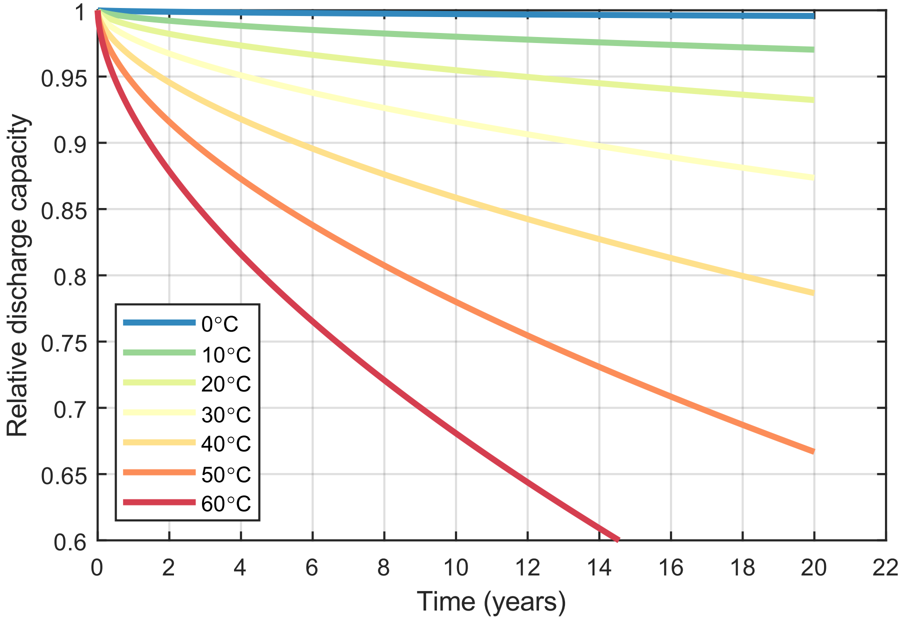
Gasper, P., Gering, K., Dufek, E., Smith, K. *J. Electrochem.* ***2021****, 168(2), 020502*

Model extrapolation to 20 years

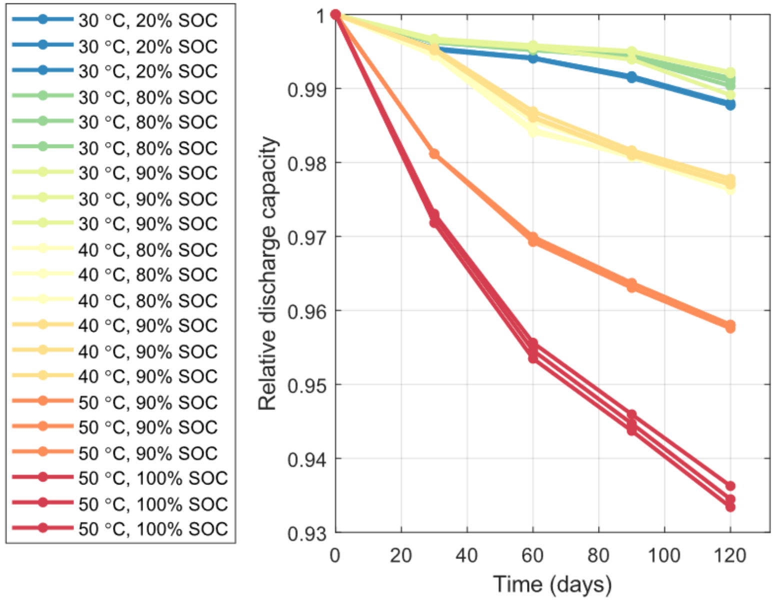
- Auto-generated models reduce time needed for predictions.
- Realistic Model predictions for T based on collection of 4-5 months of data.
- Full design of experiments for both calendar and cycle life using LTO/LMO cells

Simulation (0.5 C_{rate}, 100% DOD)

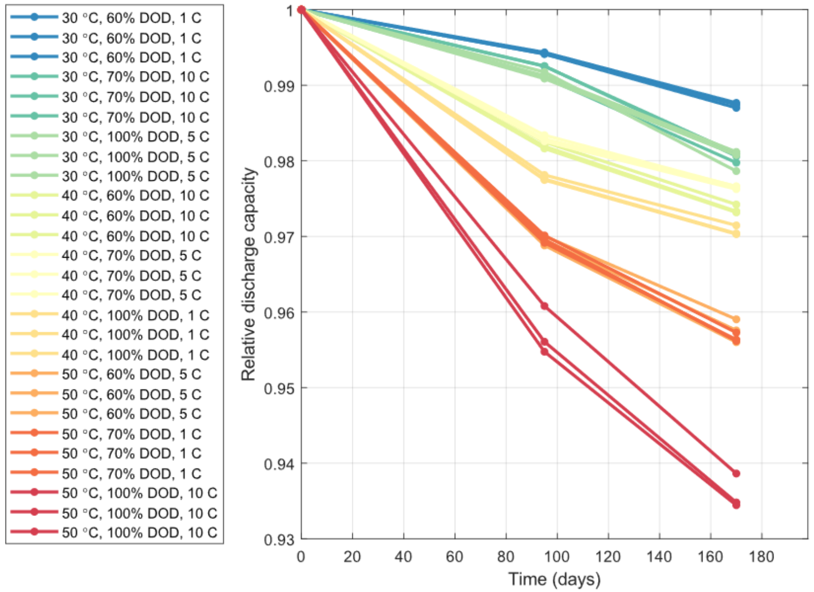
14600 EFC (2 EFC/day or 33% duty cycle)



Calendar aging

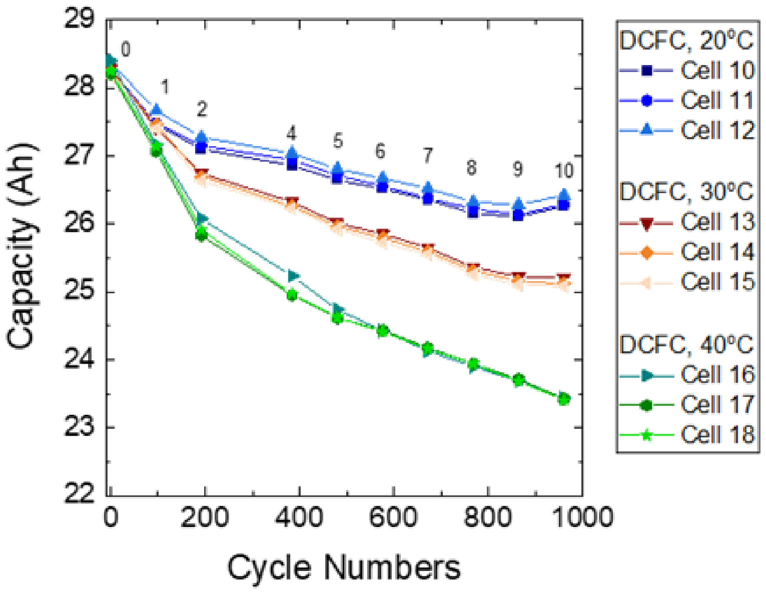


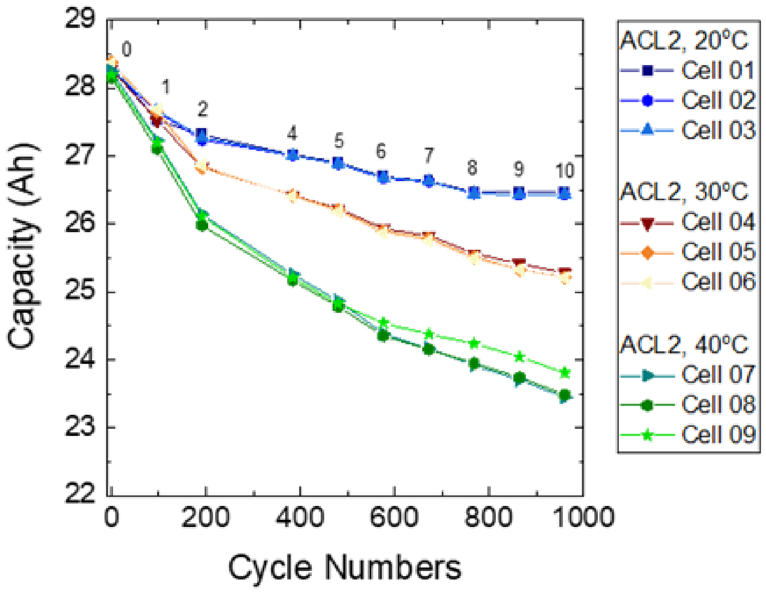
Cycling aging

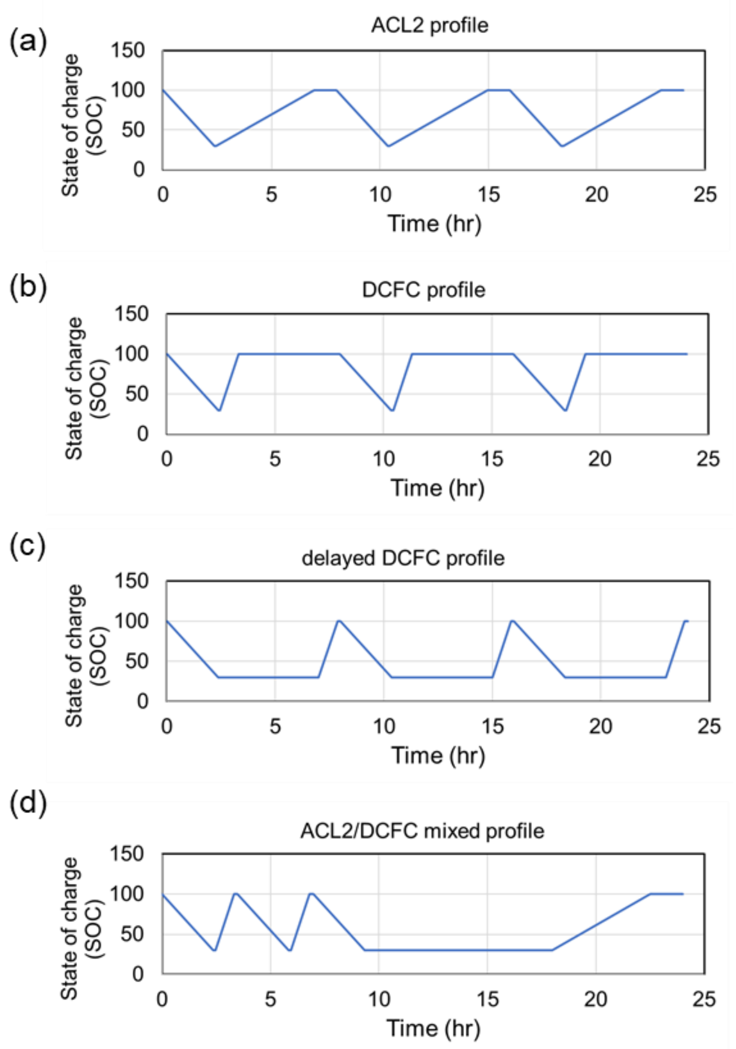


Understand the degradation from fast charging

- Comparison of AC Level 2 and DCFC
- Mixed use profiles
- Delayed DCFC protocol reduces capacity fade up to 1.3% at RPT9 compared to no delay DCFC
- Nissan Leaf Cells (and aligned pack data)



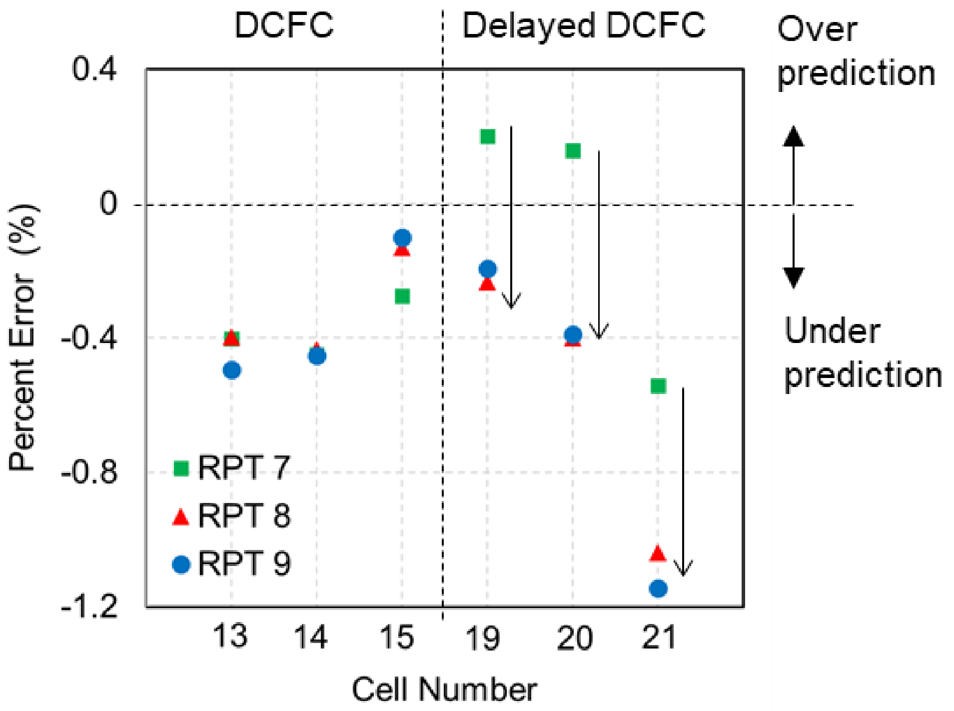




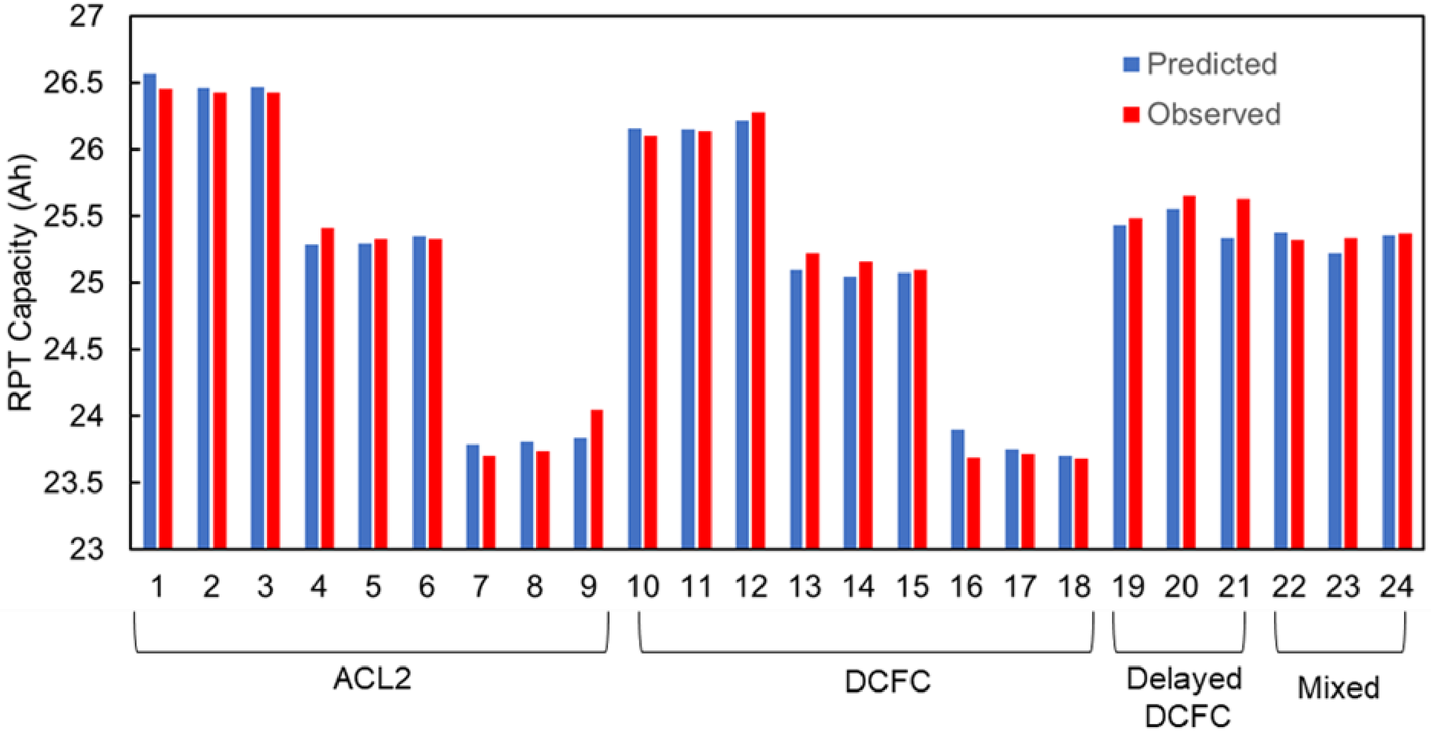
T. Tanim et. al, J. Power Sources **2018**, 381, 56
Kunz et al, Batteries & Supercaps, **2021** doi.org/10.1002/batt.202100079

RPT capacity projection

- Using existing data it is possible to predict capacity at 864 cycles using the first 45 DST cycles - ~5% of data acquired for mixed use conditions
- But, data-driven and even physics-based techniques will fail if calendar considerations aren't evolved
- Use of cycling only data provides low error, but overprediction of fade for mild calendar conditions



Overprediction of fade for mild calendar conditions



Kunz et al, Batteries & Supercaps, **2021** doi.org/10.1002/batt.202100079

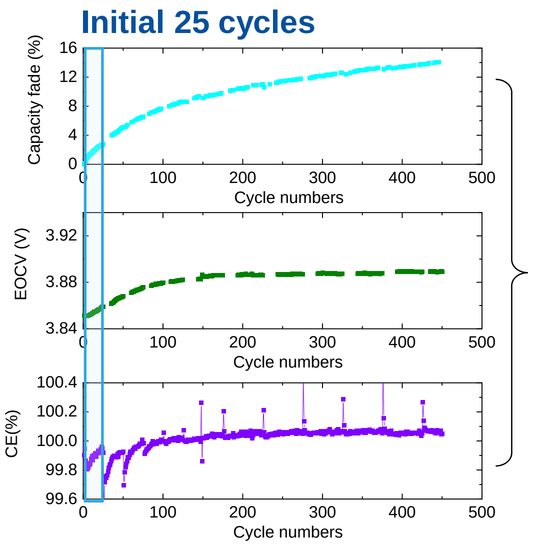
Constructing an algorithm that separates Li-plating and SEI

Physically meaningful electrochemical signatures

Capacity fade

End of charge voltage

Coulombic efficiency



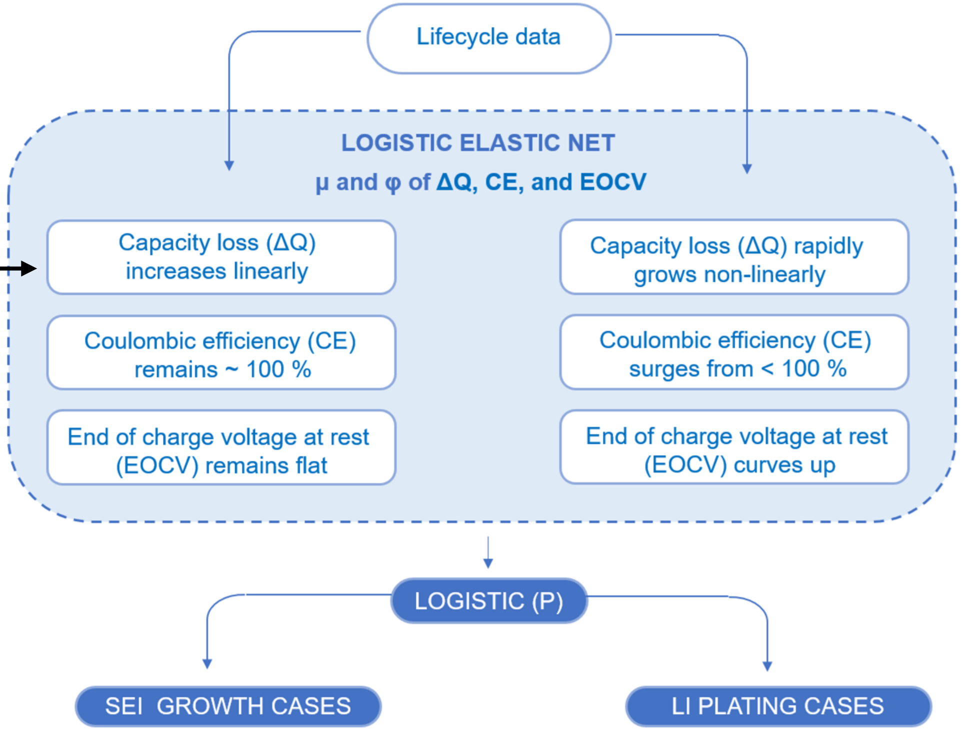
ML classification Logistic elastic net

Mean (μ) → initial state

Autoregressive (φ) → time dependence

Correlation between coherent EC signatures

Decision making procedure (classification of cells)



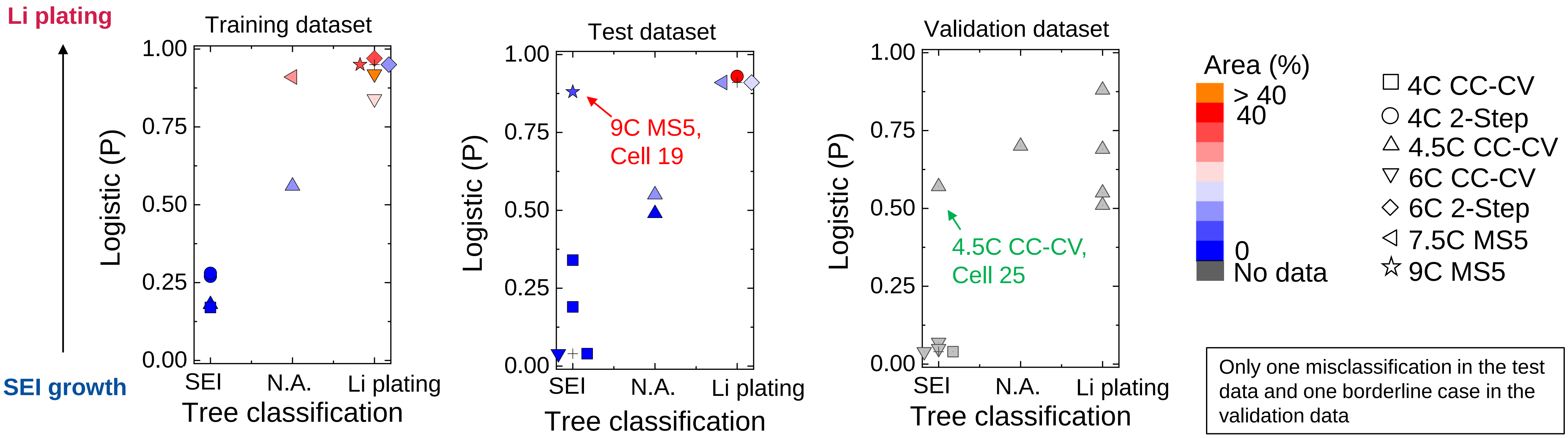
	Charging protocols	Cell numbers
P1	4C CC-CV*	01, 02, 03
	4C 2-step**	04, 05, 06
	4.5C CC-CV	07, 08, 09
	6C CC-CV	10, 11, 12
	6C 2-step	13, 14, 15
	7.5C MS5***	16, 17
	9C MS5	18, 19
P2	4.5C CC-CV	20, 21, 22
		23, 24, 25
P3	4C CC-CV	26, 27
	6C CC-CV	28, 29, 30, 31

31 NMC/graphite cells:
Training: known condition
Test: known condition
Validation: *unknown* condition

Chen et al., *Cell Reports Physical Science*, ***2021***, *2(3)*, 100352

Classifying likelihood of Li plating

- Multiple signatures have coherent response – need to be considered jointly
- Aligning signatures into a decision framework enhances ability to readily encompass in a ML framework
- Analysis can use 25 cycles or less vs 100+ for human evaluation
- ***First step toward ability to predict life and failure mode – Tailored cell engineering for cost reduction***



Only one misclassification in the test data and one borderline case in the validation data

Chen et al., *Cell Reports Physical Science*, ***2021***, *2(3)*, 100352

Remaining challenges and barriers

- Alignment of data quantity, quality and availability
  - Not all data created equal
- Joint prediction of life and performance for both standard and non-typical use cases
  - Based on accelerated cycle and calendar aging
- Continued expansion for other chemistries
- Performance prediction using different order electrochemical models
- Joint use of experimental and synthetic data
- Expanded data needs and coordination of tools for data quality evaluation

Proposed Future Research

- Continued expansion and inclusion of additional failure modes and prediction schemes
- Expanded synthetic data generation
- Coordinated data sharing across multiple national laboratories and other institutions
- Aligned electrochemical and life models with incorporated failure mode analysis

Any proposed future work is subject to change based on funding levels

Contributors and Collaborators

Collaborations: Behind-the-meter-storage (bat442) and XCEL (bat456-463)

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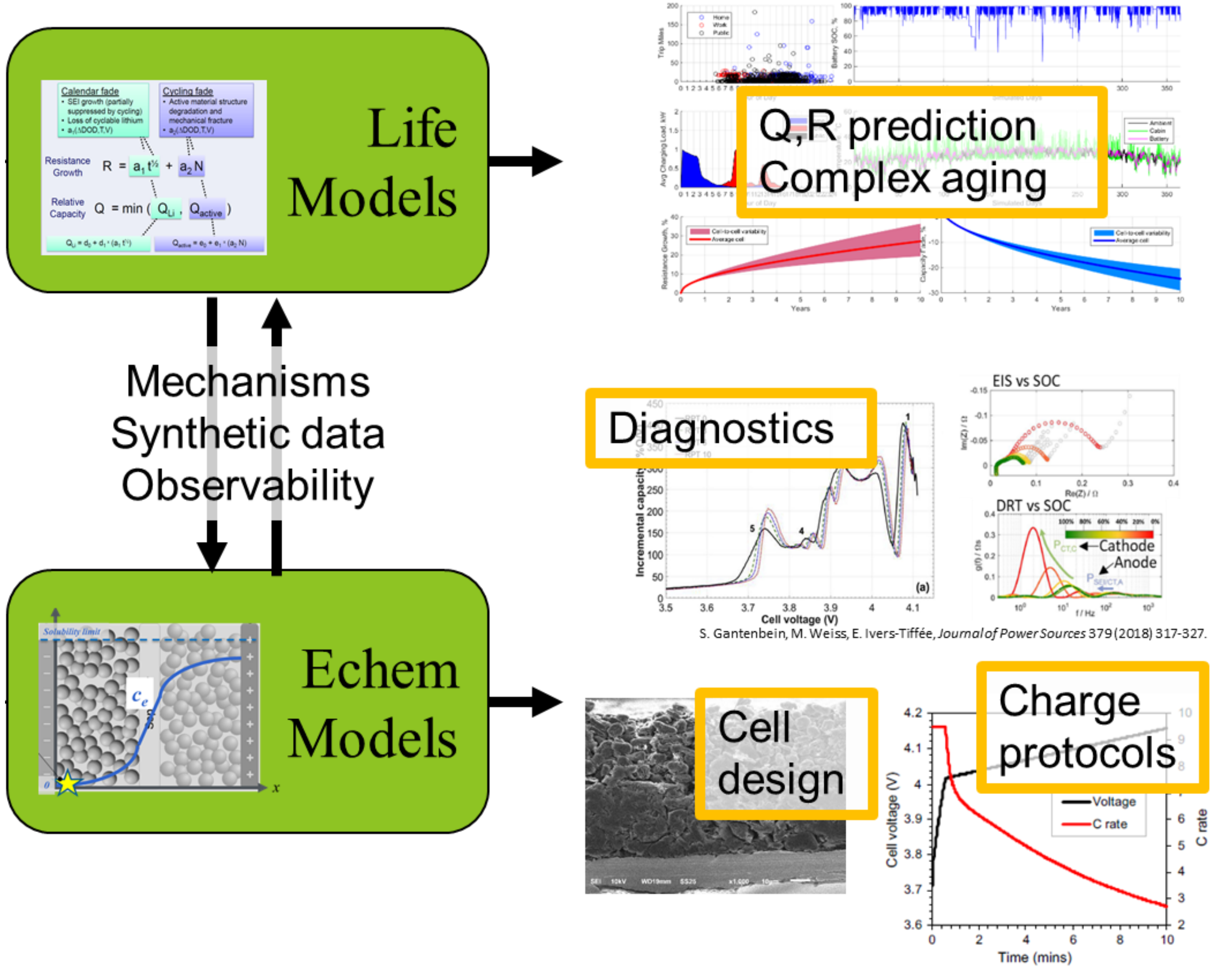
University of Oxford
Carnegie Mellon University
Toyota Research Institute
University of Washington
Sandia National Laboratories
RWTH Aachen University
HNEI Hawai'i Natural Energy Institute, University of Hawai'i at Mānoa

Summary

- Autogeneration of life models reduces time for life predictions
- Early life prediction possible using 2 weeks of cycling data
- Methods can be extended to non-training data streams
- Identified EC signatures that physically correlated to SEI or Li plating
- Established an ML classification framework that classifies aging modes
- Using multiple signatures decision can be made early, within the first 25 life cycles



Acknowledgements

We thank **Simon Thompson, Samuel Gillard, Steven Boyd and David Howell** for VTO programmatic support. **Tony Burrell and Venkat Srinivasan** for coordination on BTMS and XCEL projects

Cells were provided by Cell Analysis, Modeling, and Prototyping (CAMP) facility at Argonne National Laboratory.

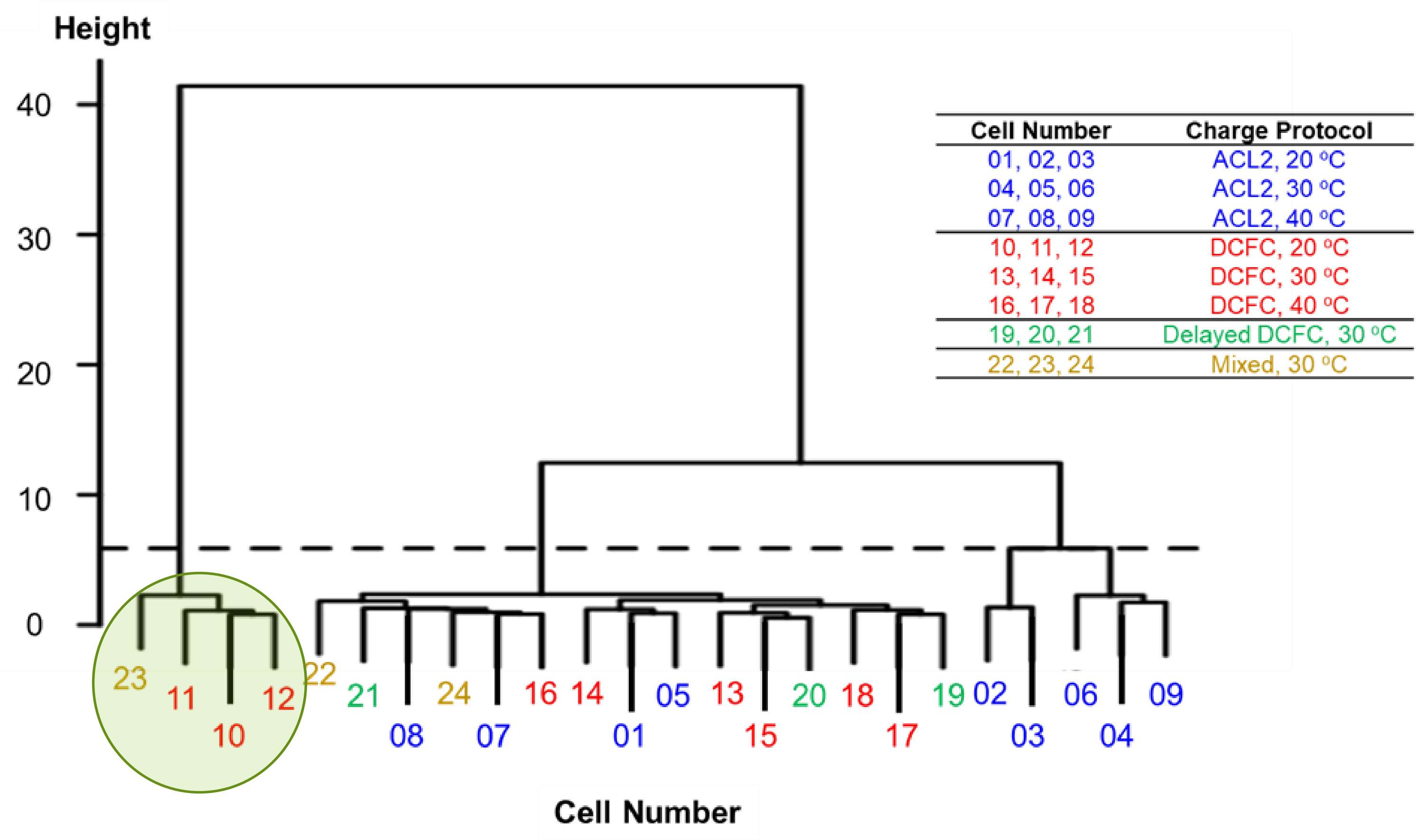
Reviewer Only Slides

Publications

- B.R. Chen, M.R. Kunz, T.R. Tanim, E.J. Dufek "A machine learning framework for early detection of lithium plating combining multiple physics-based electrochemical signatures" *Cell Reports Physical Science*, 2(3) 100352 (2021) doi.org/10.1016/j.xcrp.2021.100352
- P. Gasper, K. Gering, E. Dufek, K. Smith "Challenging practices of algebraic battery life models through statistical validation and model identification via machine-learning" *J. Electrochem. Soc.* 168(2), 020502 (2021) doi.org/10.1149/1945-7111/abdde1
- M.R. Kunz, E.J. Dufek, Z. Yi, K.L. Gering, M.G. Shirk, K. Smith, B.R. Chen, Q. Wang, P. Gasper, R.L. Bewley, T.R. Tanim "Early battery performance prediction for mixed use charge profiles using hierarchal machine learning" *Batteries & Supercaps* (2021), in press https://doi.org/10.1002/batt.202100079
- L. Ward, S. Babinec, E.J. Dufek, D.A. Howey, V. Viswanathan et al "Principles of the Battery Data Genome" *submitted*
- S. Kim, Z. Yi, B.R. Chen, T.R. Tanim, E. Dufek "A Deep Learning Modeling Framework for Early Classification and Quantification of Lithium-ion Aging Modes" *submitted*

Robust Analysis

- Capture and analyze what effects noise and outliers have on the prediction
  - Necessary in linking to Physics Based Models
  - Asses if more samples are needed
  - Understand variation trends
- Applied ML algorithms:
  - Time series outlier detection
  - Prototypical Clustering



Kunz et al, submitted

Supervised forecast algorithm examples

Q – capacity during constant power portion of charge (kinetic)

V (EOC) – after rest to link with thermodynamic change

T – skin T tracked, followed environmental chamber

A R I MA auto-regressive integrated moving average

auto-regressive

$$y_t = c + \phi_1 y_{t-1} + \phi_2 y_{t-2} + \cdots + \phi_p y_{t-p} + \varepsilon_t,$$

forecast the variable of interest (y) at time point t using a linear combination (φ) of past values ($y_{t-1} \ldots y_{t-p}$) of the variable. However, battery degradation is usually non-linear.

moving average

$$y_t = c + \varepsilon_t + \theta_1 \varepsilon_{t-1} + \theta_2 \varepsilon_{t-2} + \cdots + \theta_q \varepsilon_{t-q},$$

uses past forecast errors (ε) in a regression-like model.

$$y'_t = c + \phi_1 y'_{t-1} + \cdots + \phi_p y'_{t-p} + \theta_1 \varepsilon_{t-1} + \cdots + \theta_q \varepsilon_{t-q} + \varepsilon_t,$$

Input:	x: experimental response for Q_{cp}, EOCV and T, y: RPT capacity at end of life
1.	for Each predictor by cycle do
2.	Treat outliers within time series
3.	Application of ARIMA
4.	Reform predictors as X
5.	Hierarchical clustering on each cell within X
6.	Ridge regression on RPT using DST
7.	Generalized Adaptive LASSO with RR coefficients

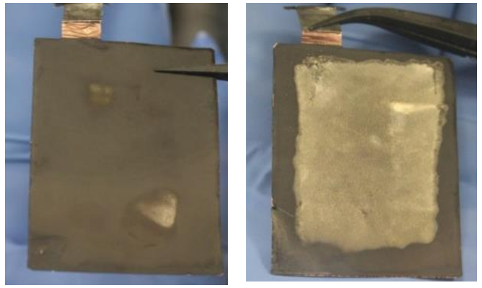
https://otexts.com/fpp2/

31 fast charging NMC532/Gr pouch cells

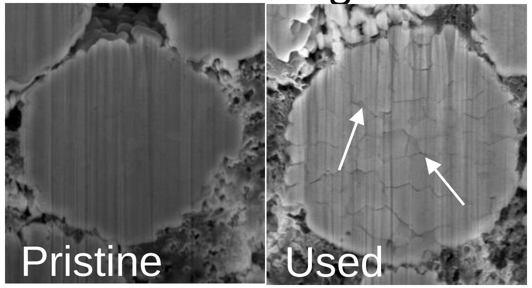
Cell design group	Charging protocols	Cell numbers	Anode loading	Anode porosity
P1	4C CC-CV* 4C 2-step** 4.5C CC-CV 6C CC-CV 6C 2-step 7.5C MS5*** 9C MS5	01, 02, 03 04, 05, 06 07, 08, 09 10, 11, 12 13, 14, 15 16, 17 18, 19	9.94 $mg.cm^{-2}$	34.5%
P2	4.5C CC-CV	20, 21, 22	9.94 $mg.cm^{-2}$	22.3%
		23, 24, 25	9.94 $mg.cm^{-2}$	49.1%
P3	4C CC-CV 6C CC-CV	26, 27 28, 29, 30, 31	6.38 $mg.cm^{-2}$	37.4%

Major aging phenomena

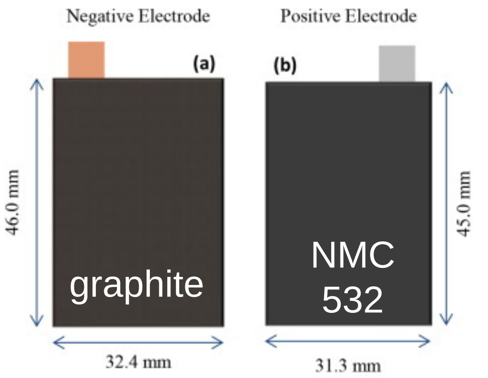
Li plating



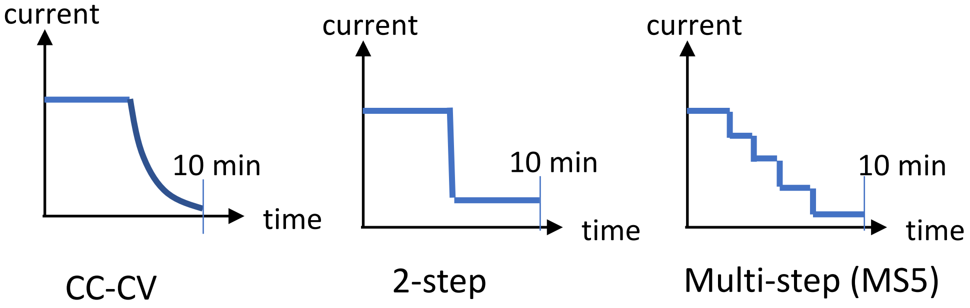
Cathode cracking



Cell architecture



Charging protocols (time = 10 mins)



XCEL
eXtreme Fast Charge Cell Evaluation of Lithium-ion Batteries

T. Tanim *et al.*, *J. of Electrochemical Soc*. (2019), A1926