
# Mechanistic Li-Ion Battery Modeling, What's Next?

**Matthieu Dubarry & David Beck**

matthieu@hawaii.edu


UH Materials Science Consortium for Research and Education CoRE

School of Ocean and Earth Science and Technology, University of Hawai'i at Mānoa

HNEI Hawai'i Natural Energy Institute, University of Hawai'i at Mānoa

# Mechanistic Li-Ion Battery Modeling, What's Next?

## Objectives and motivations

Early development in mid 2000s by Bloom *et al.* and Honkura *et al.* along with differential voltage analysis.

- Conceptually based on early traditional physics-based modeling studies
- Less calculation-intensive while still providing material insights

Detailed frameworks available since 2012 (Smith *et al.*, Dubarry *et al.*)

- Ease diagnosis of commercial Li-ion batteries
- Enable prognosis

Approach well validated for low rate constant current data

- Degradation modes quantification
- Plating identification
- Knee forecasting

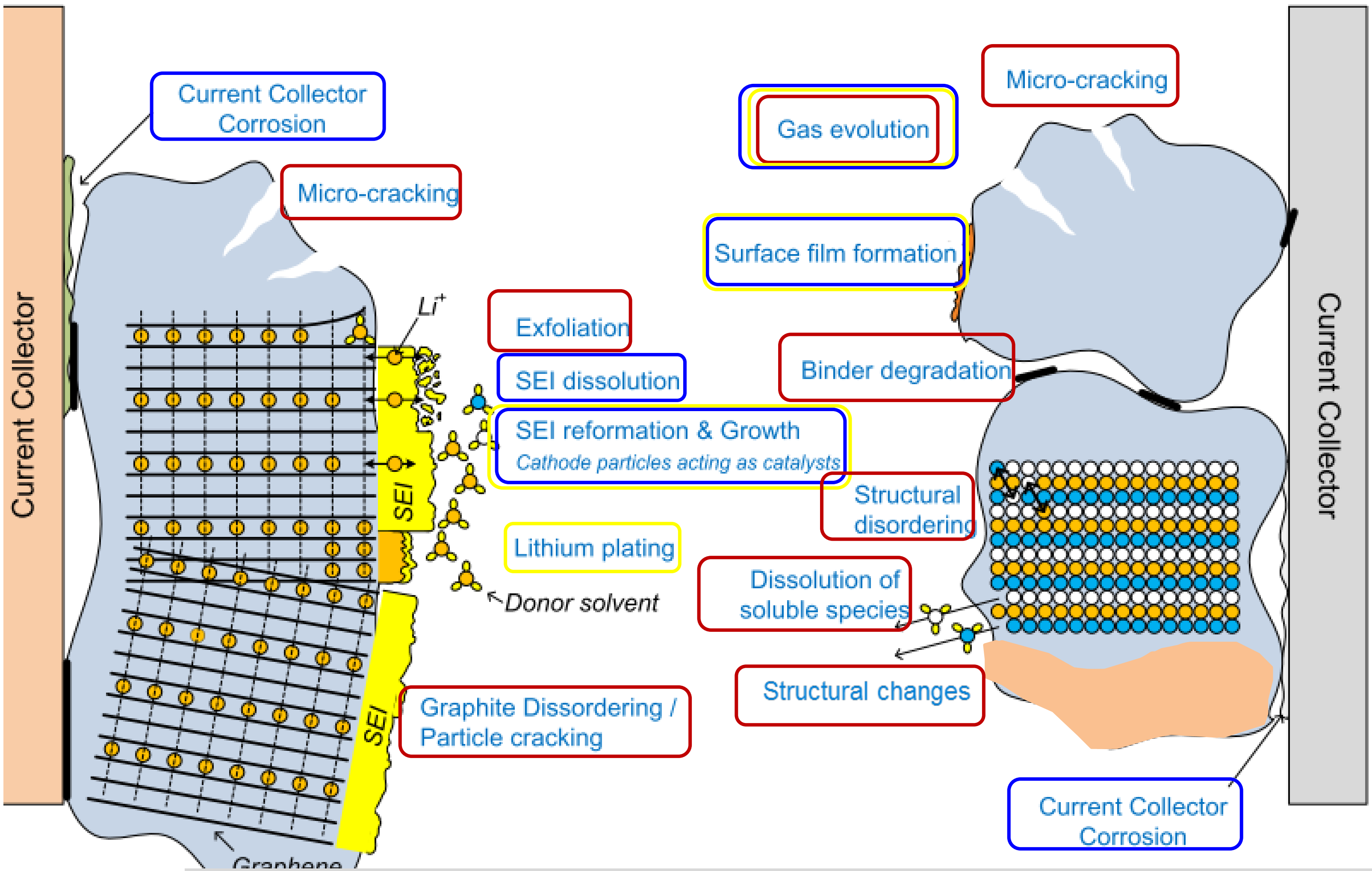
But some limitations remains

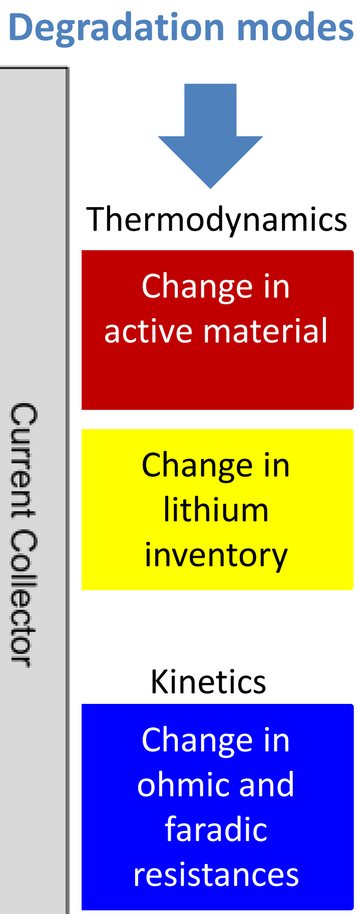
- Faster rates, blends, inhomogeneities, non-constant current cycles…

**This work proposes possible directions to improve the framework**

# Multiple mechanisms to consider

## Lithium ion battery degradation mechanisms




Degradation modes refer to **the impact of a mechanism rather than its root cause.**



M. Dubarry, C. Truchot and B.Y. Liaw, *J.Power Sources*, **219** (2012) 204-216

# Mechanistic modeling

## General Principles

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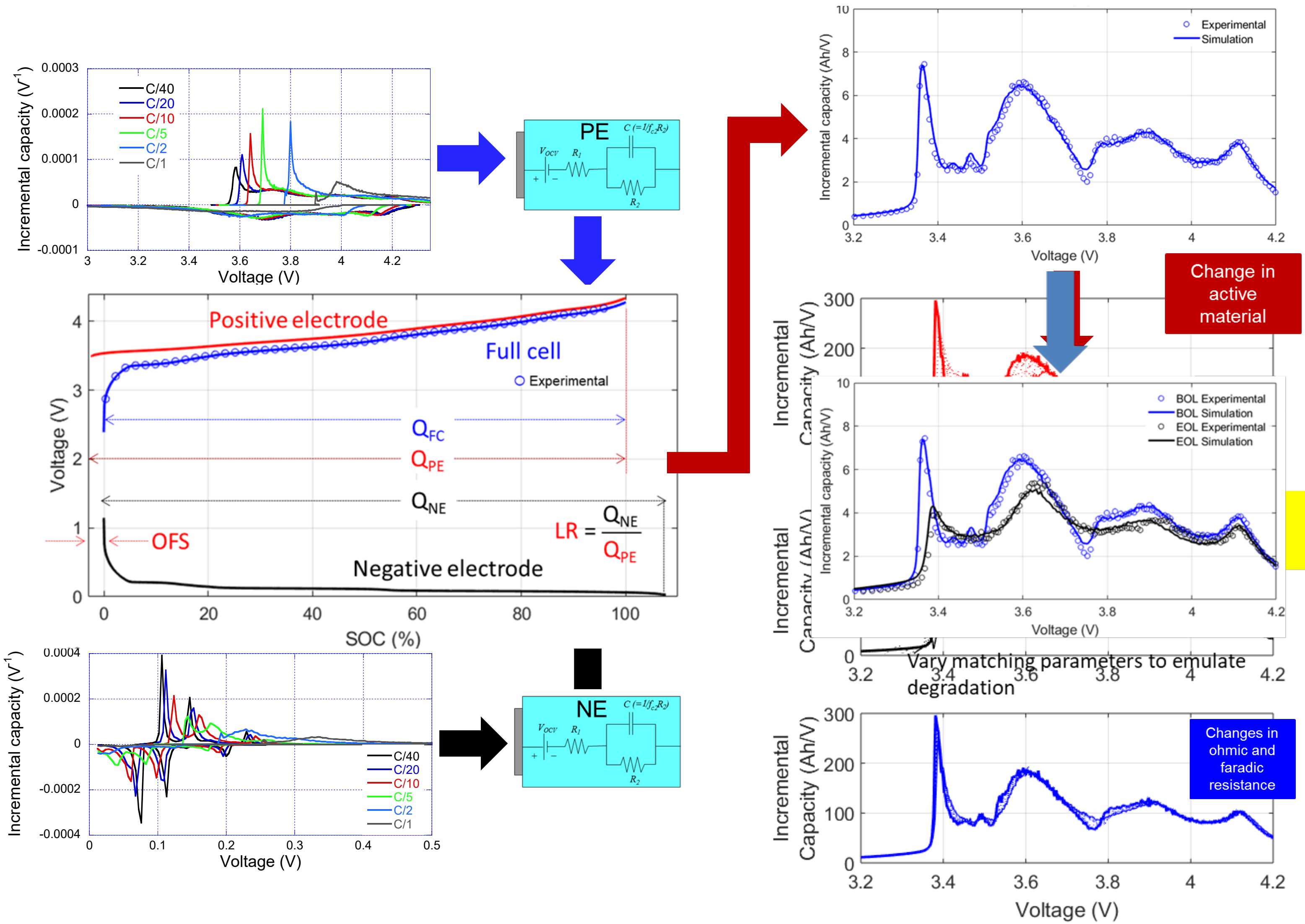
## Loss of lithium inventory (LLI) & Loss of Active Material (LAM)

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# Mechanistic modeling
## General Principles

Change in ohmic and faradic resistances

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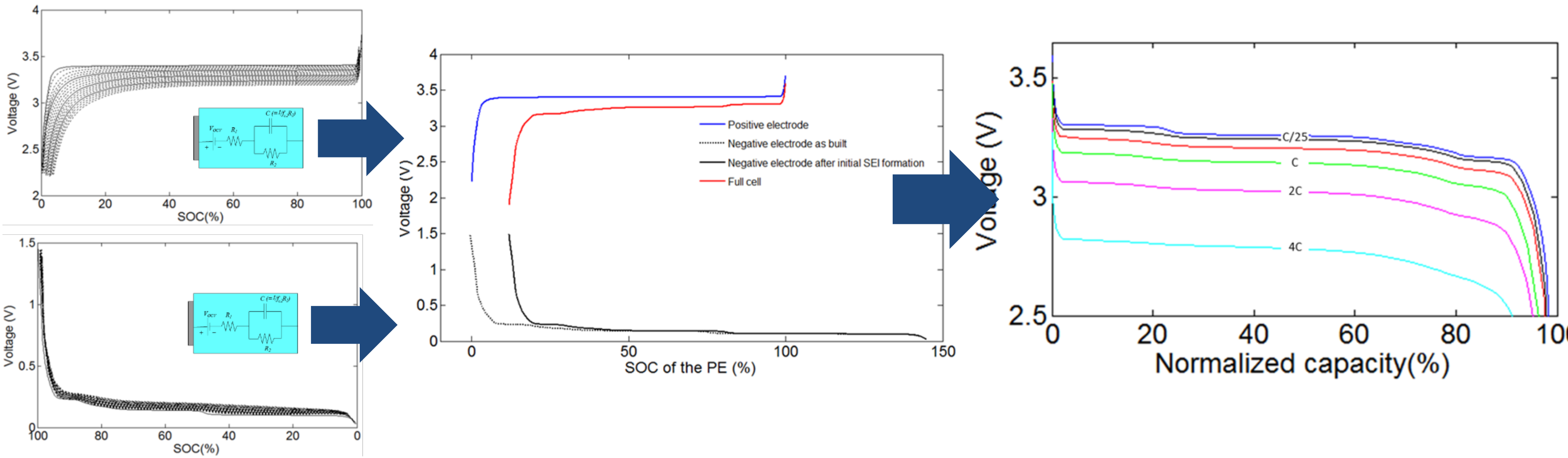
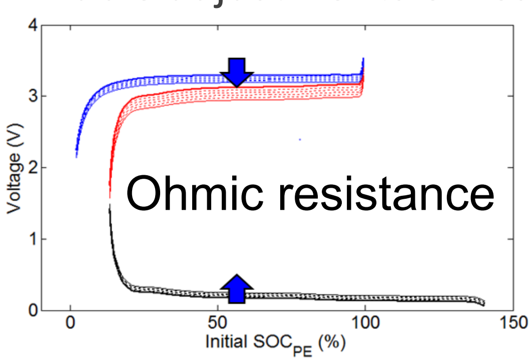
## Emulating resistive and kinetic changes: Emulate effect of current

### From Half cell data at different rates

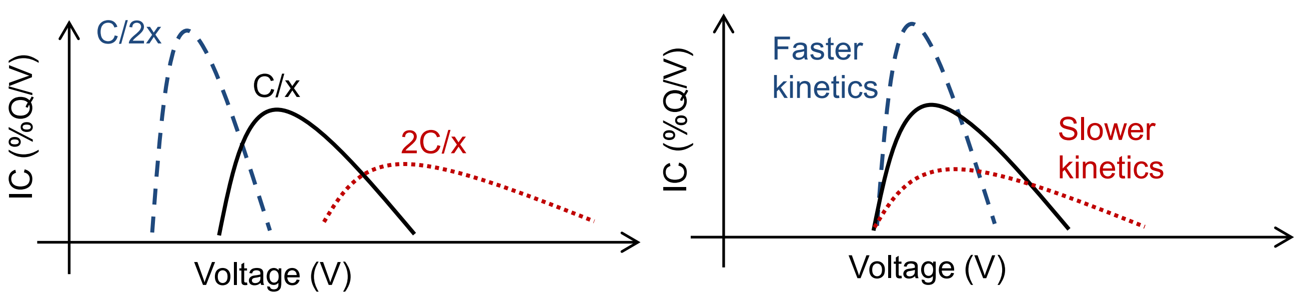
Use ECM to calculate voltage response at every possible rate




Enable adjustments of resistance and kinetics




Faradic resistance






M. Dubarry, C. Truchot and B.Y. Liaw, *J.Power Sources*, **219** (2012) 204-216

# Mechanistic modeling

## General Principles

Change in ohmic and faradic resistances

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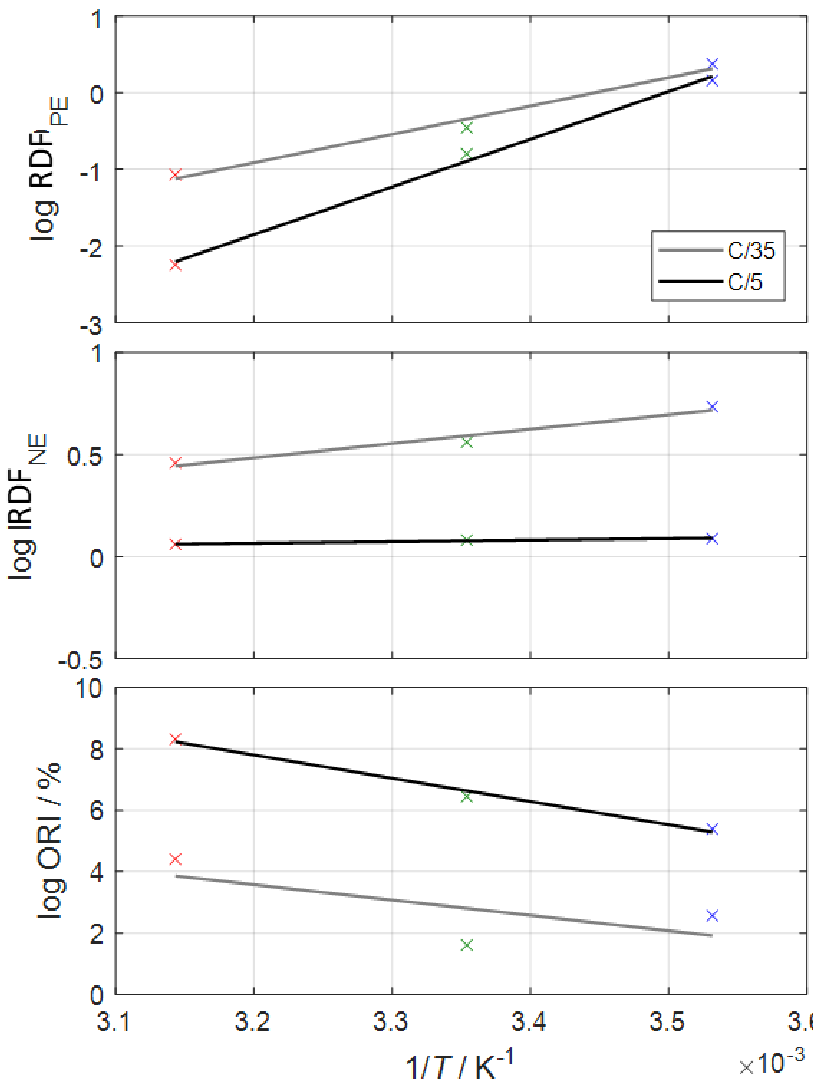
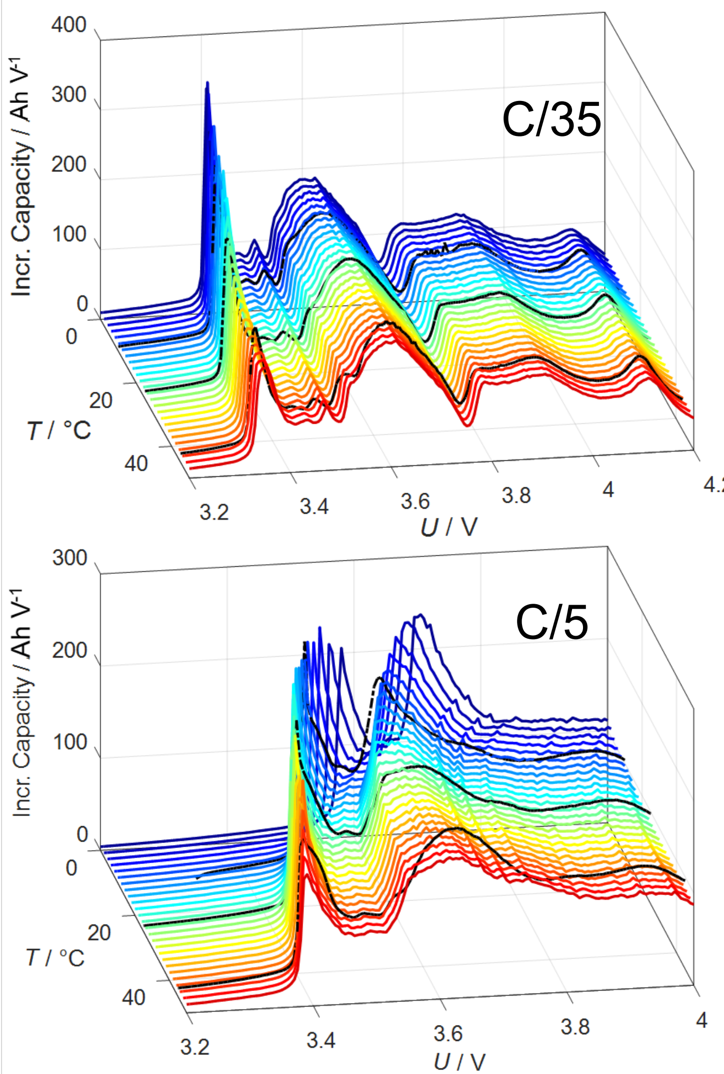
### Kinetics






Schindler, S., et al. (2019). "Kinetics accommodation in Li-ion mechanistic modeling." Journal of Power Sources **440**: 227117.

# Mechanistic modeling
## General Principles

Change in active material

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### Blending

#### Initial approach

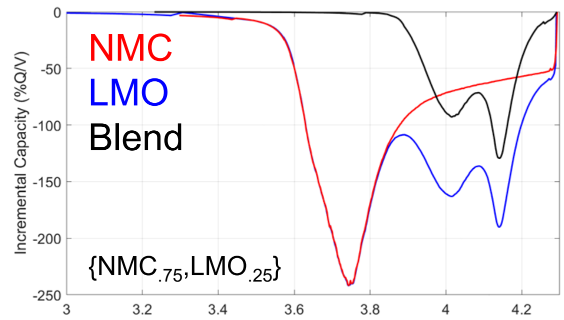
Not taking current distribution in consideration

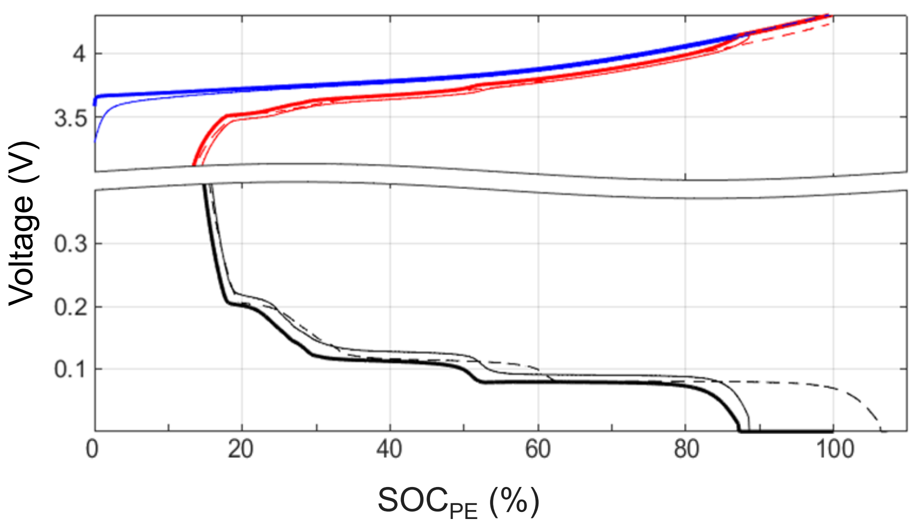
### Lithium Plating

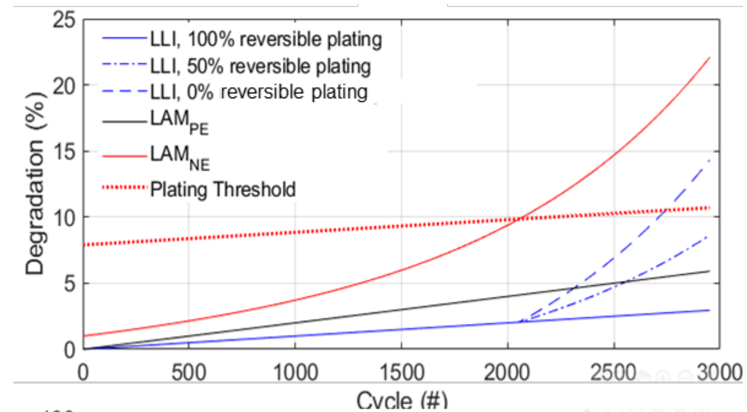
#### Add Li metal as active material when needed

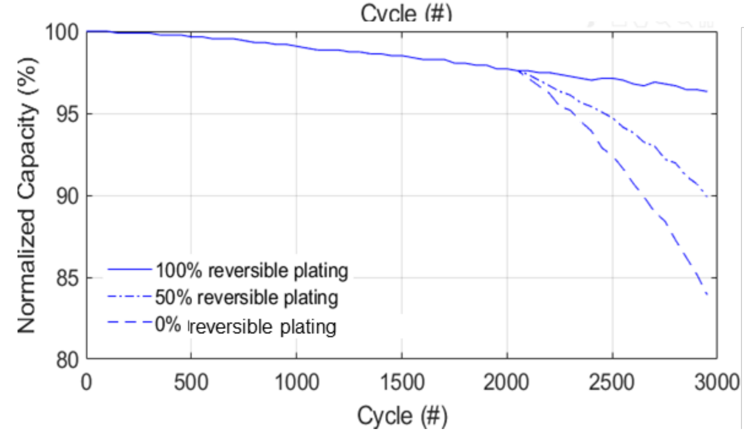
Allow Knee simulation and prediction

LAM, Rate capability, or resistance based






Dubarry M. et al., Journal of Power Sources 479 (2020) 228806
Dubarry M. and D. Beck, Accounts of Material Research, 10.1021/accountsmr.2c00082

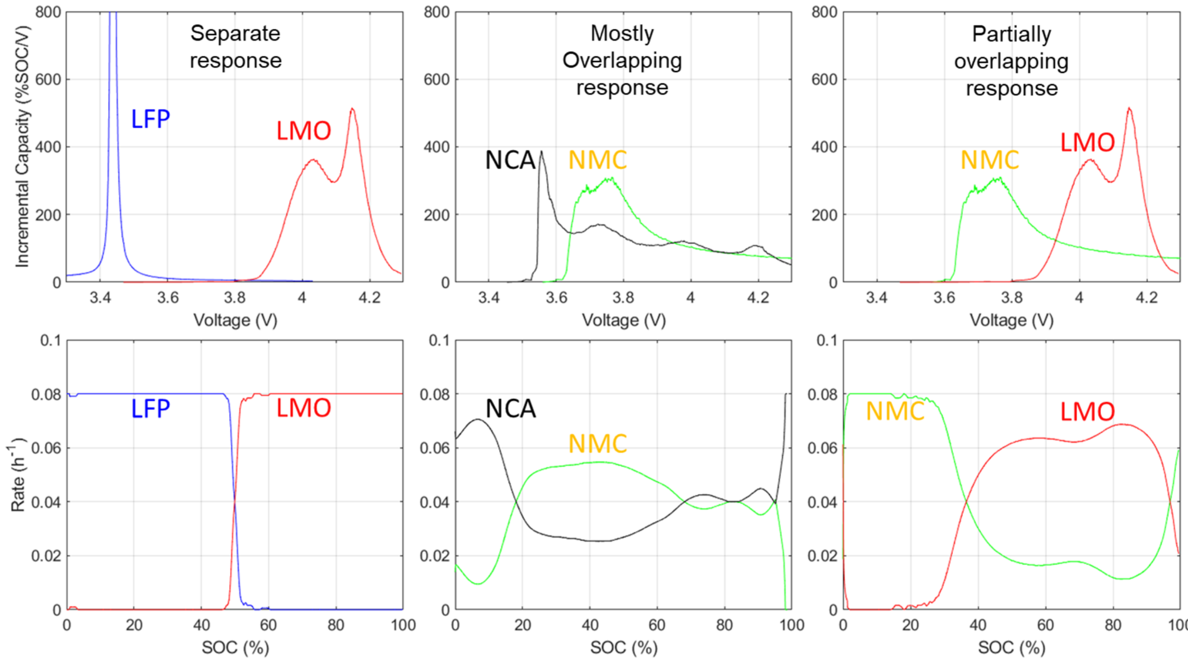
# Mechanistic modeling

## General Principles

### Blending – What's next

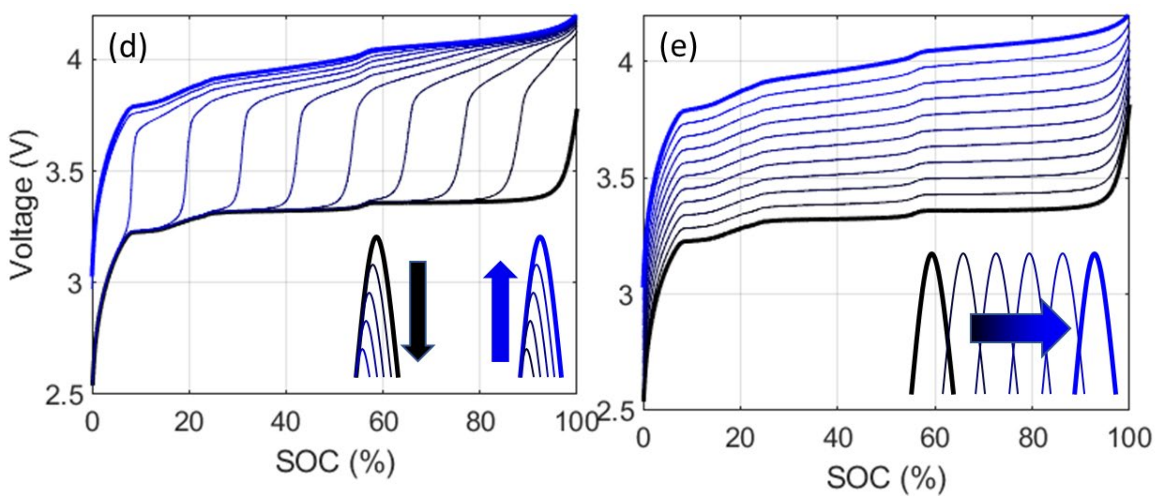
Need for a paralleling model

- Take current distribution into
- Consideration
- Uses simulation at different rates




### Voltage fade

- Phase transformation
- Solid Solution

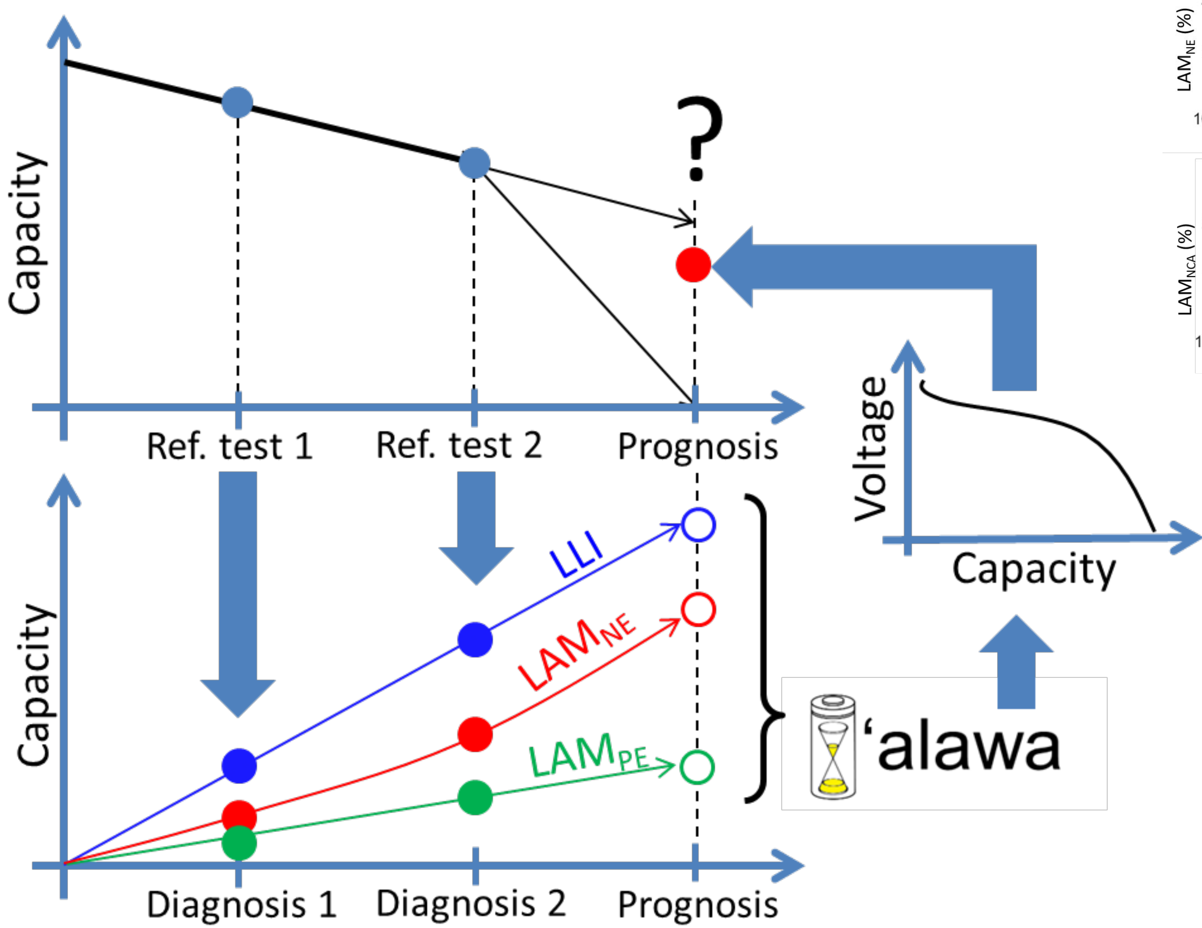


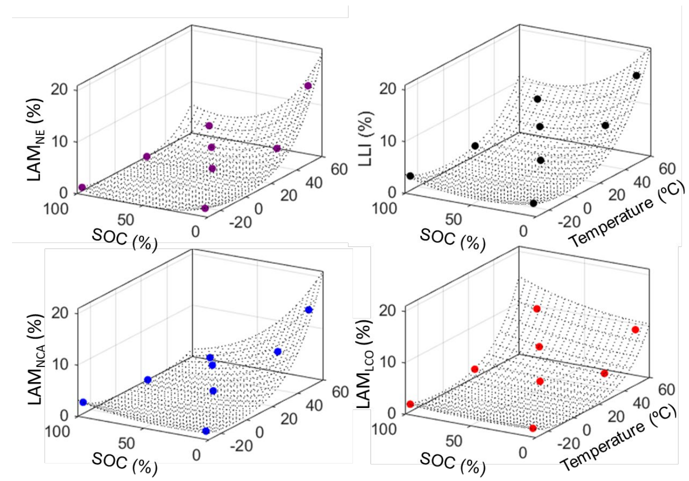


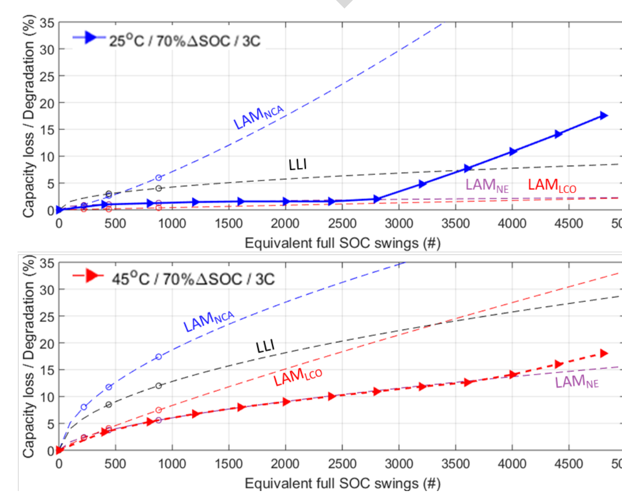

Heubner, C.; Liebmann, T.; Schneider, M.; Michaelis, A. Electrochim. Acta 2018, 269, 745-760, doi:10.1016/j.electacta.2018.02.165c
Dubarry M. and D. Beck, Accounts of Material Research, 10.1021/accountsmr.2c00082

# Mechanistic modeling
## General Principles

### From diagnosis to prognosis






*Journal of The Electrochemical Society*, **166** (10) A1991-A2001 (2019)

# Mechanistic modeling
## Prospective Features

### Inhomogeneities

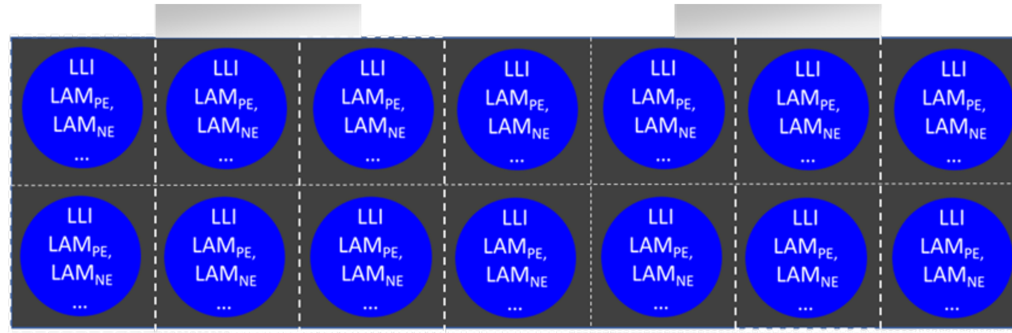
Uses simulations at diff. rates

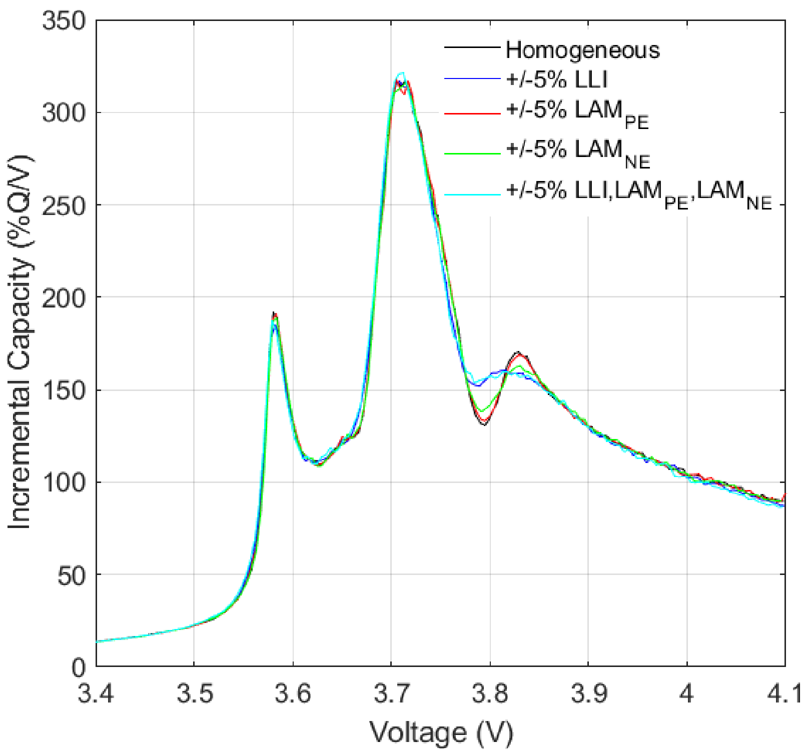
Uses paralleling model

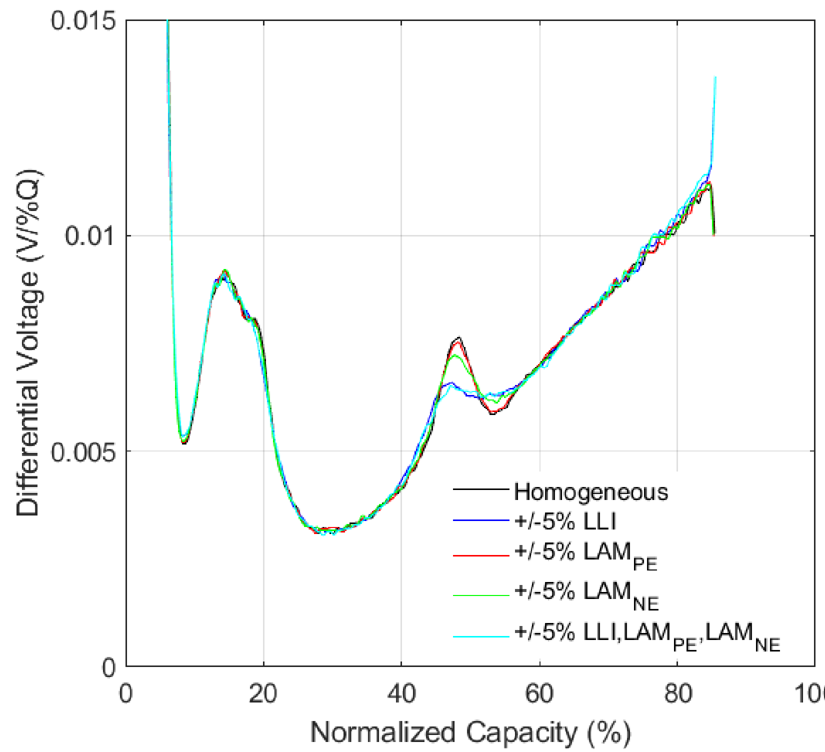
For modules

For large electrodes

Possible Li transfer between segments





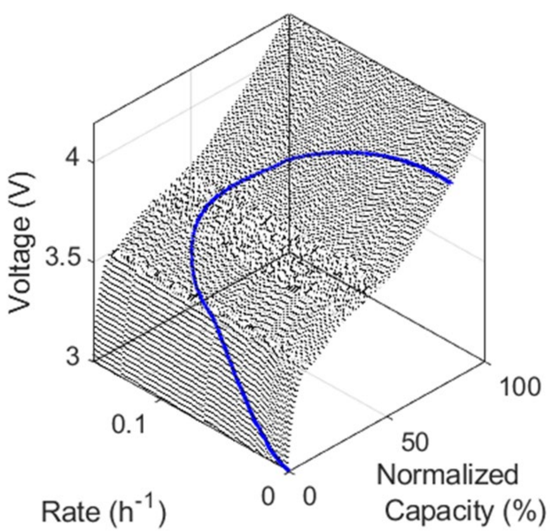

Dubarry M. and D. Beck, Accounts of Material Research, 10.1021/accountsmr.2c00082

# Mechanistic modeling
## Prospective Features

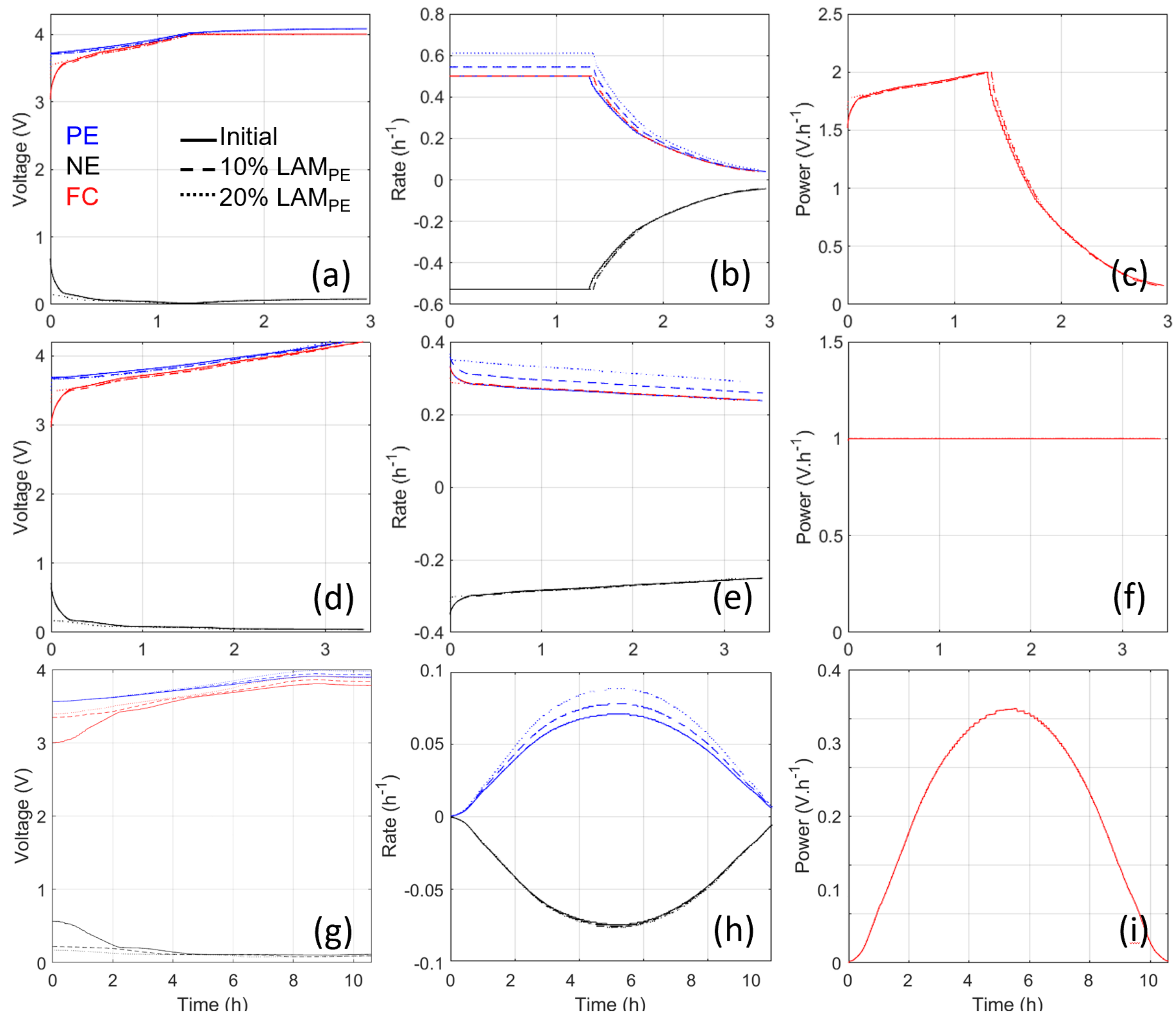
### Complex duty cycles

Uses simulations at diff. rates

Uses  paralleling model




Poster A-2466 Data-Driven Direct Diagnosis of PV Connected Batteries






Dubarry M. and D. Beck, Accounts of Material Research, 10.1021/accountsmr.2c00082

Big Data for Li-Ion Diagnosis and Prognosis

# Use the mechanistic modeling approach

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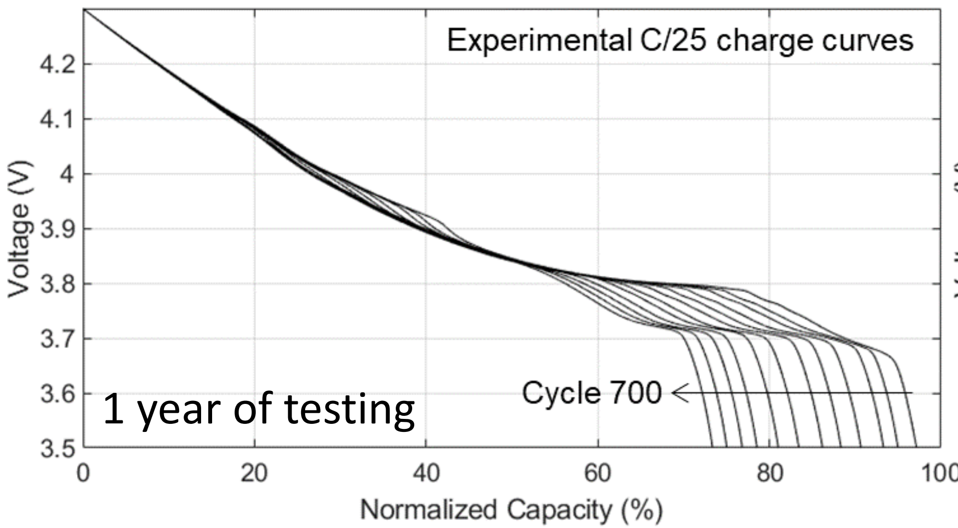
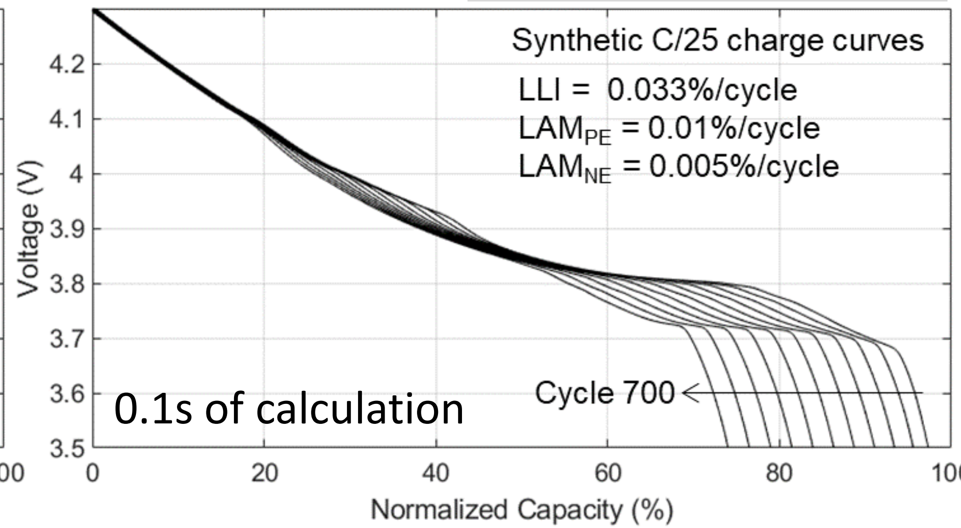
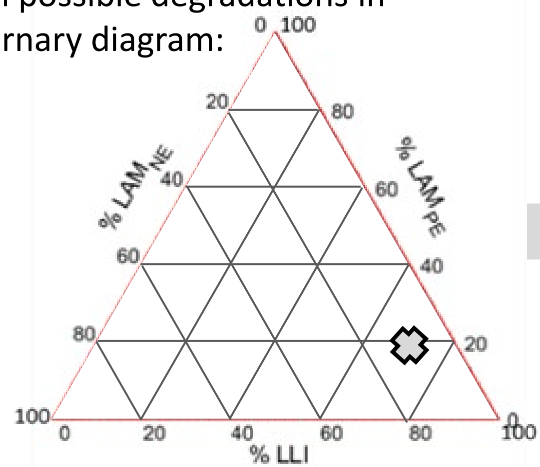
## Emulation of battery electrochemical response

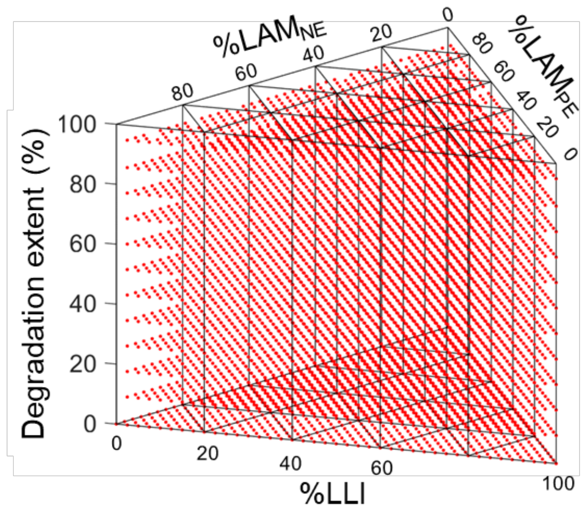
Aging reconstructed from simple equations




All possible degradations in ternary diagram:




Infinite training data for diagnosis AI algorithms

Poster A-2466 Data-Driven Direct Diagnosis of PV Connected Batteries


Dubarry M. et al., Journal of Power Sources 479 (2020) 228806, Dubarry M. et al., Energies 2021, 14, 2371. https://doi.org/10.3390/en14092371
Dubarry, M., et al. (2017). "State of health battery estimator enabling degradation diagnosis: Model and algorithm description." Journal of Power Sources **360**: 59-69.

# Li-ion batteries Digital Twins
# Mechanistic modeling

## Summary

### Validated

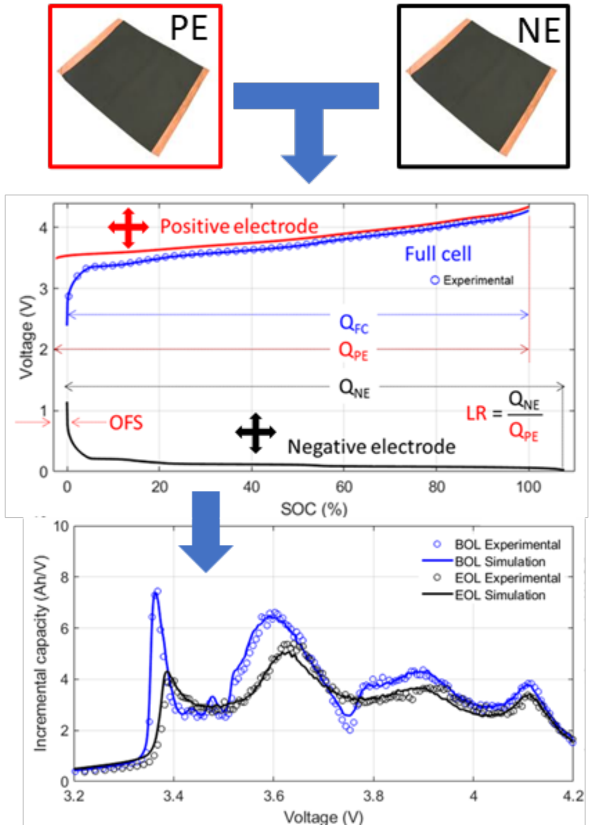
**Degradation mode diagnosis**
LLI, LAMs, Kinetics

**Material based prognosis**
With knee or not
Plating, reversible or not

**Electrochemical responses**
Constant current
Simple blends
Overdischarge
Overcharge

**Big Data**
Low rates
Feature of Interest Tracking

### Mechanistic Modeling Approach




### Under validation

**Electrochemical responses**
Na-ion and other chemistries
Advanced blends
Voltage fade
Inhomogeneous electrodes
Large battery packs
Dynamic duty cycles

**Big Data**
High rates
Temperatures
Blends
Non-continuous duty cycles



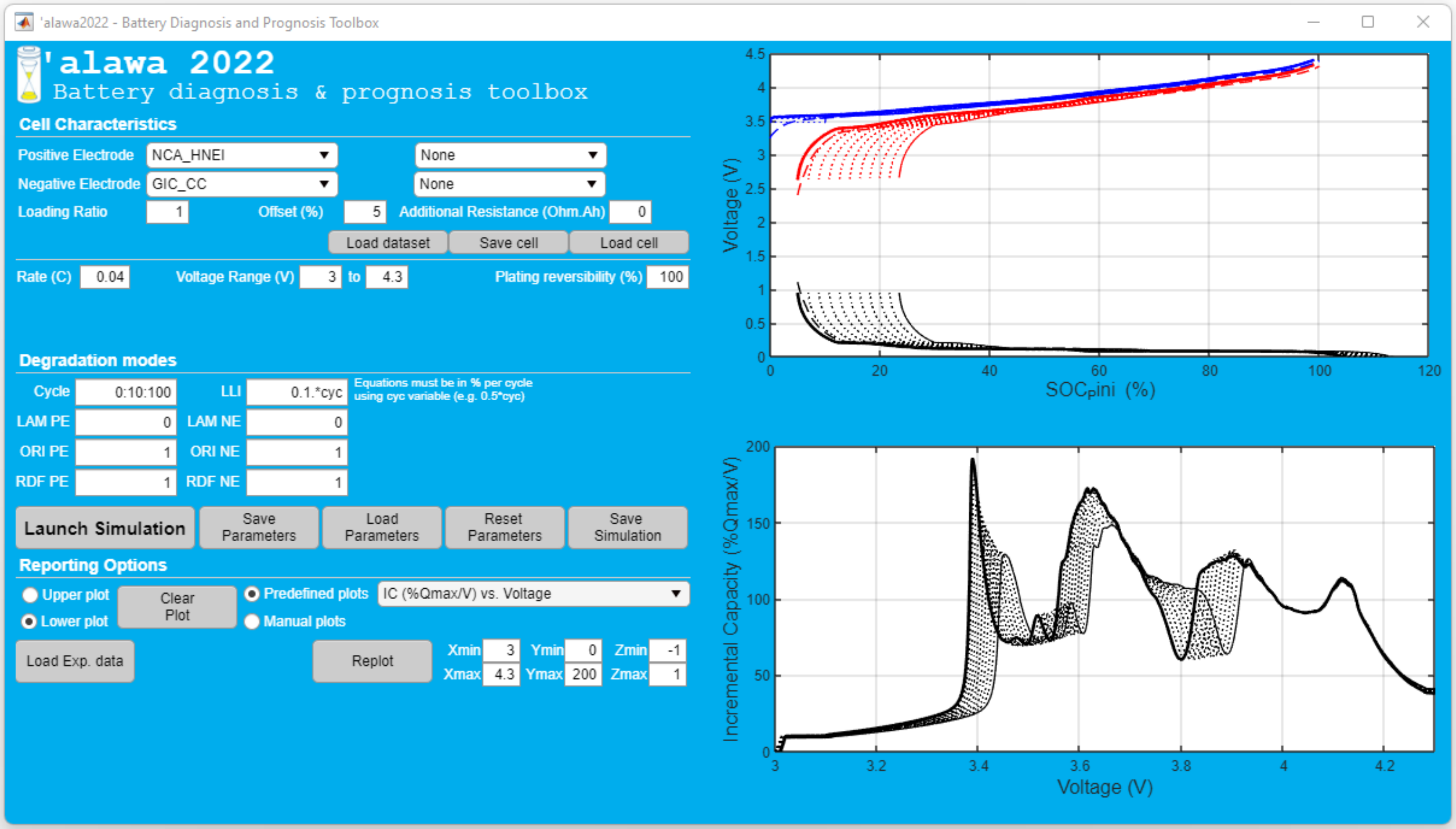

Dubarry M. and D. Beck, Accounts of Material Research, 10.1021/accountsmr.2c00082

Li-ion batteries Digital Twins

# Graphical user interface: the ‘alawa toolbox

‘alawa

## Simple, fast, powerful and accurate diagnosis and prognosis tool




Free licensing available for academic applications.

Back door access for synthetic cycles generation available with collaboration

Licensing available for industry users (GUI and backdoor)

# Acknowledgments

All my students, especially Arnaud Devie and Cyril Truchot

Current and past Funding

*Mahalo for your attention! Questions ?*

HNEI Hawai'i Natural Energy Institute
University of Hawai'i at Mānoa

matthieu@hawaii.edu