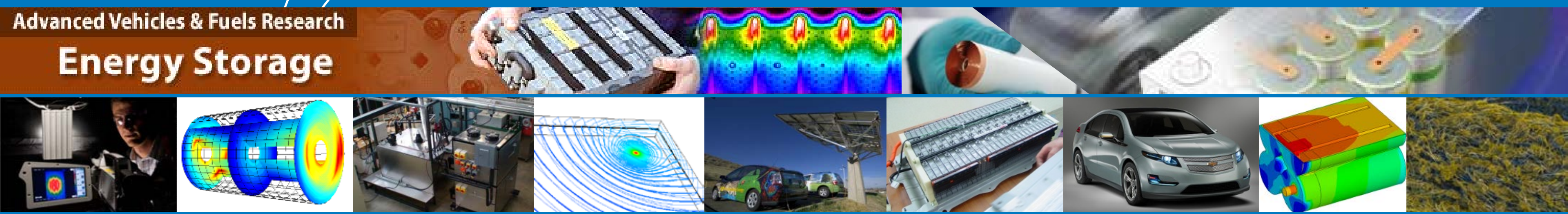
Life Prediction Model for Grid-Connected Li-ion Battery Energy Storage System



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NREL/ PR-5400-68759

Applications of Energy Storage (ES) on the Grid

Focus of present ES system life study

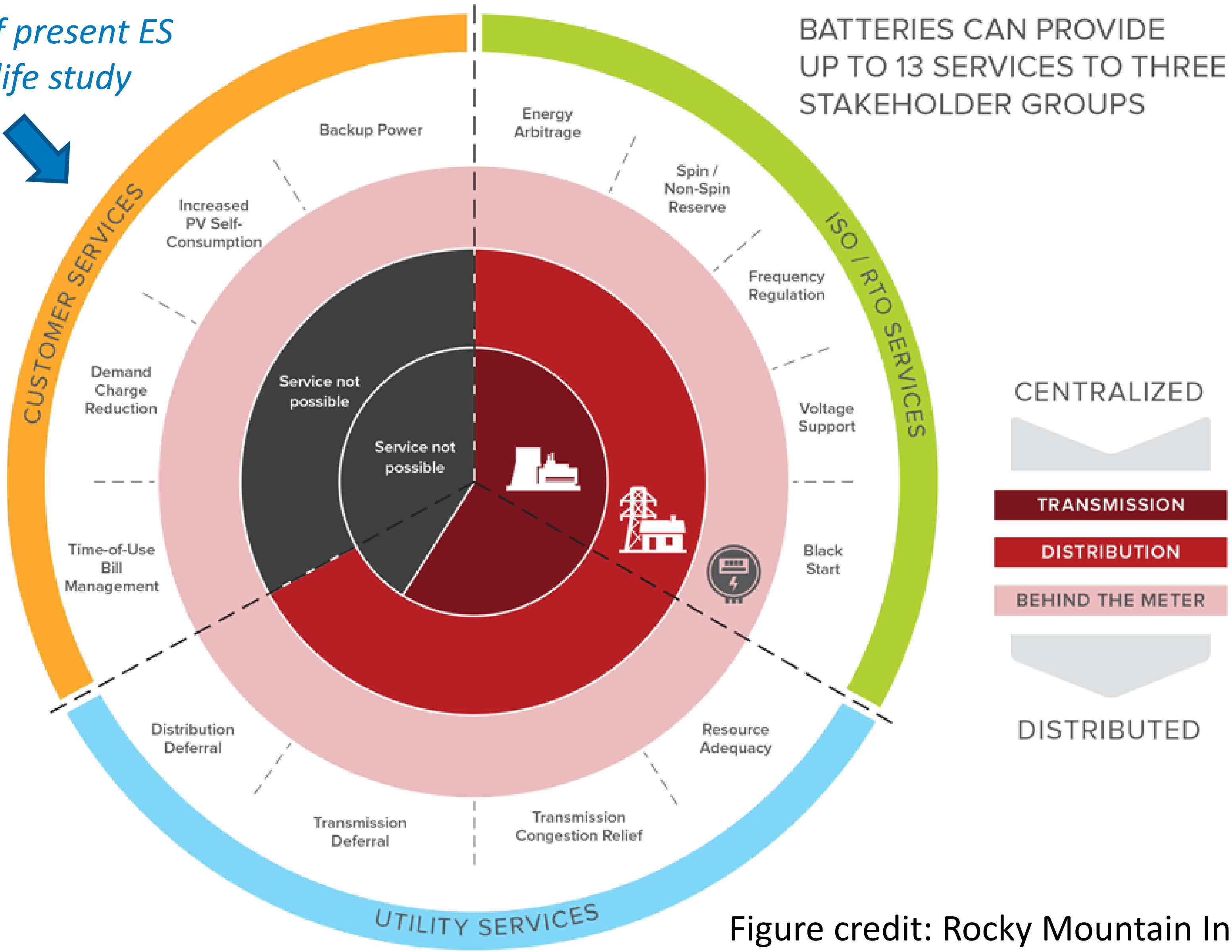


Figure credit: Rocky Mountain Institute

Example Application: Behind-the-meter ES enables PV use in locations such as Hawaii (where power export is prohibited)

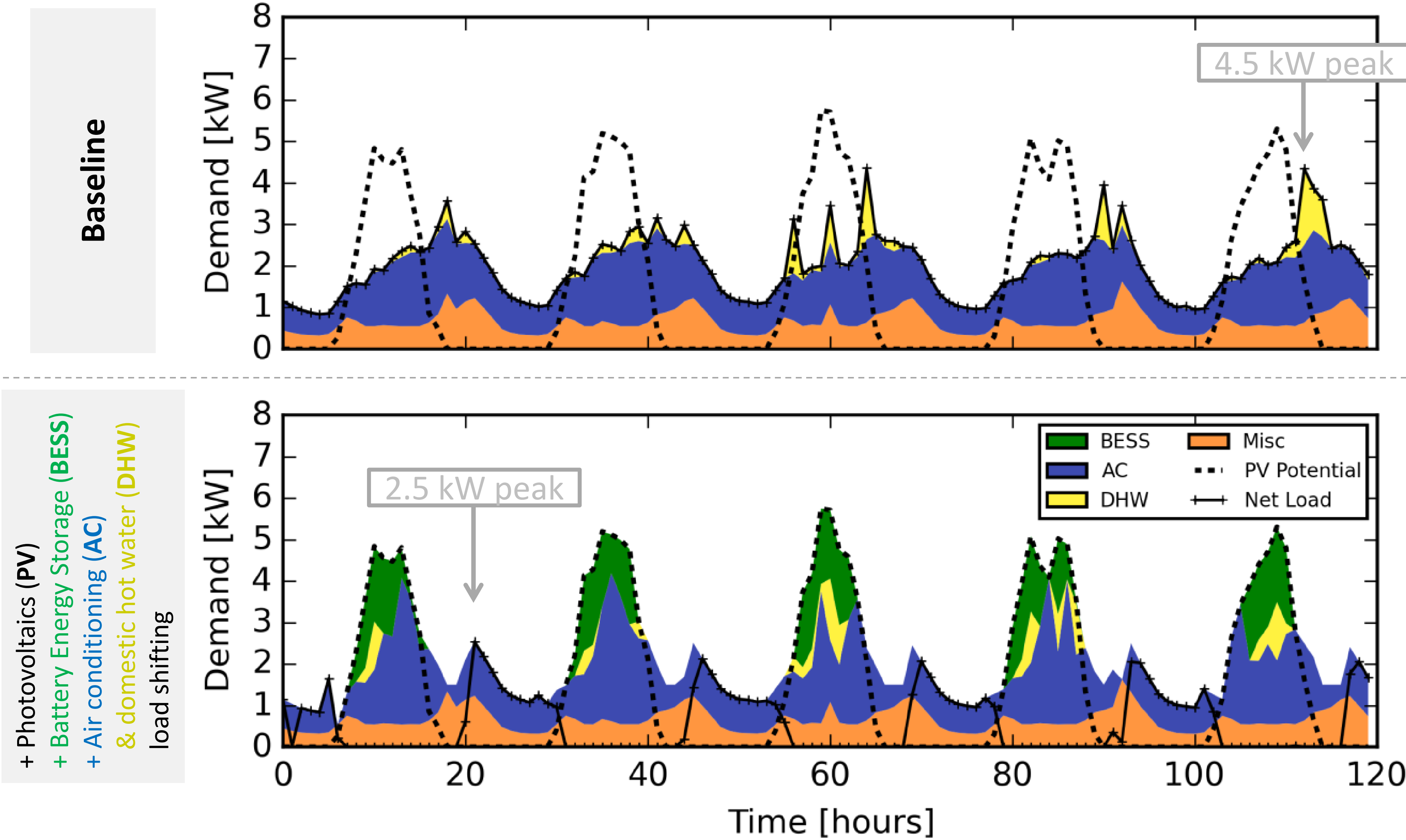


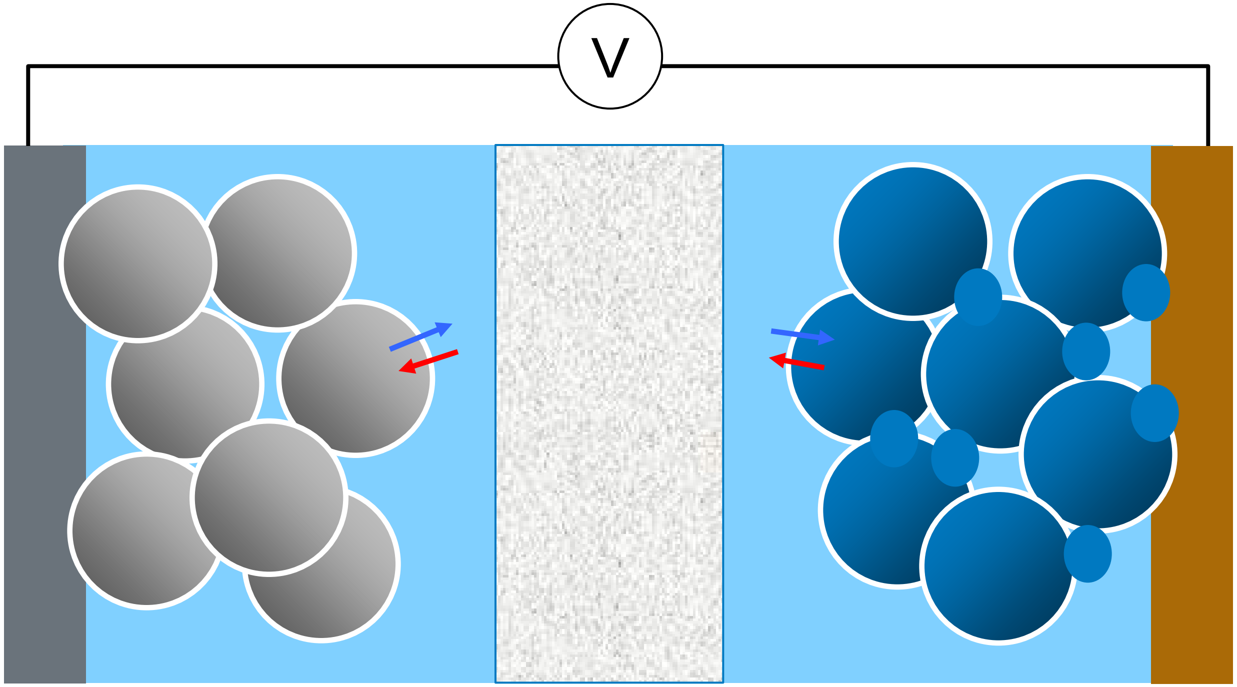
Figure: "Solar Plus: An Holistic Approach to Distributed Solar PV" Eric O'Shaughnessy, Kristen Ardani, Dylan Cutler, Robert Margolis (NREL Pub #68371)

Outline

- Degradation mechanisms
- Modeling approach
- Aging tests
- Model and parameter identification
- Example life prediction

Li-ion Working Principles

<u>Neg. Electrode</u>
Graphite
Hard carbon
Silicon
Titanate
Li metal



<u>Pos. Electrode</u>
$LiXO_2$,
X = NiMnCo
Co
NiCoAl
$LiMn_2O_4$,
$LiFeP0_4$

Figure credit: Gi-Heon Kim

Electrochemical Operating Window

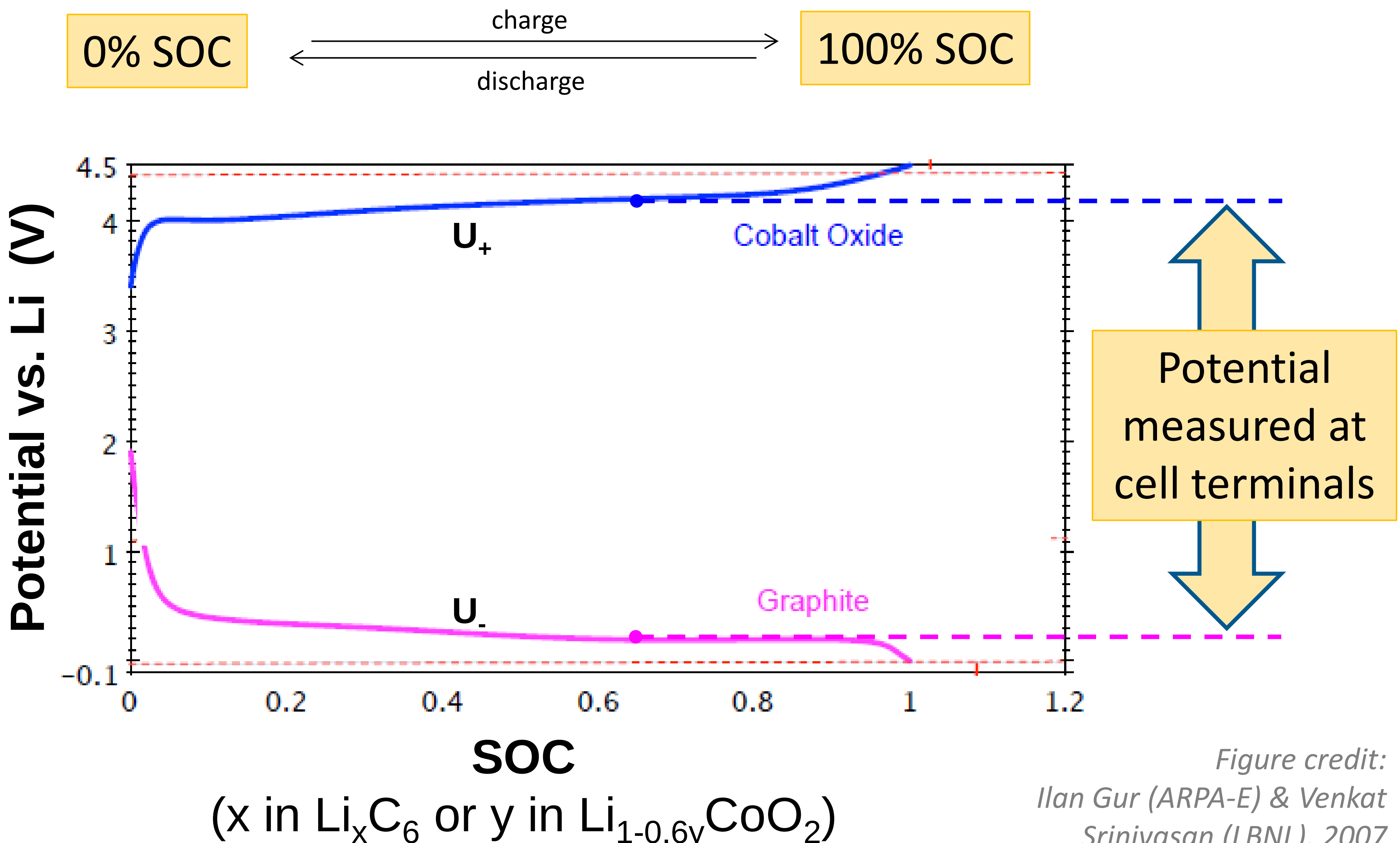
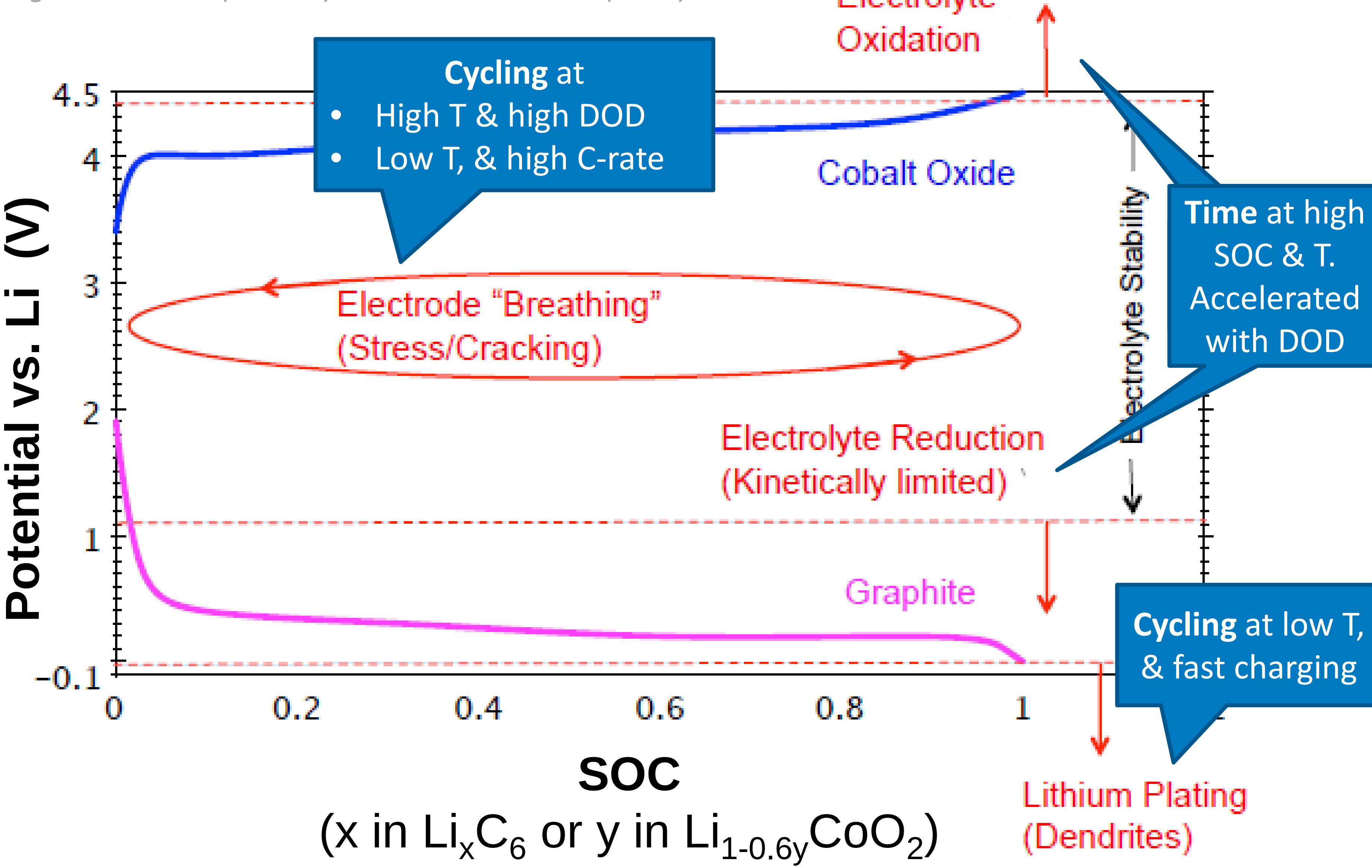


Figure credit: Ilan Gur (ARPA-E) & Venkat Srinivasan (LBNL), 2007

Electrochemical Window – Degradation

Figure : Ilan Gur (ARPA-E) & Venkat Srinivasan (LBNL) 2007



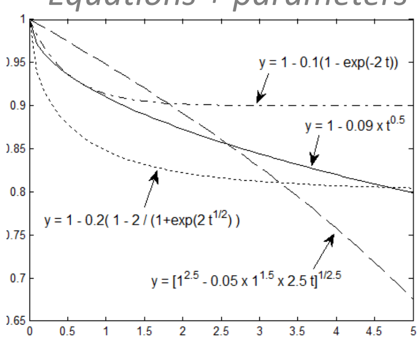
NREL Battery Life Predictive Model Framework

Reduced-order models for physical fade mechanisms, e.g.

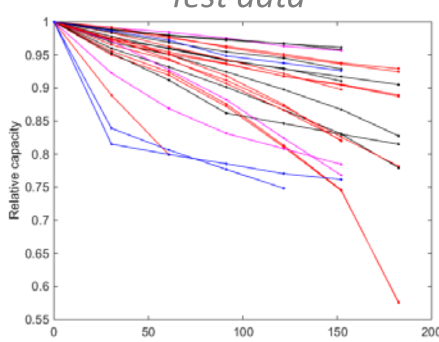
- SEI growth & damage
- Particle fracture
- Electrode isolation
- Electrolyte decomposition
- Gas generation, delamination
- Li plating

Semi-automated software aids model equation selection and parameter identification

Equations + parameters



Test data



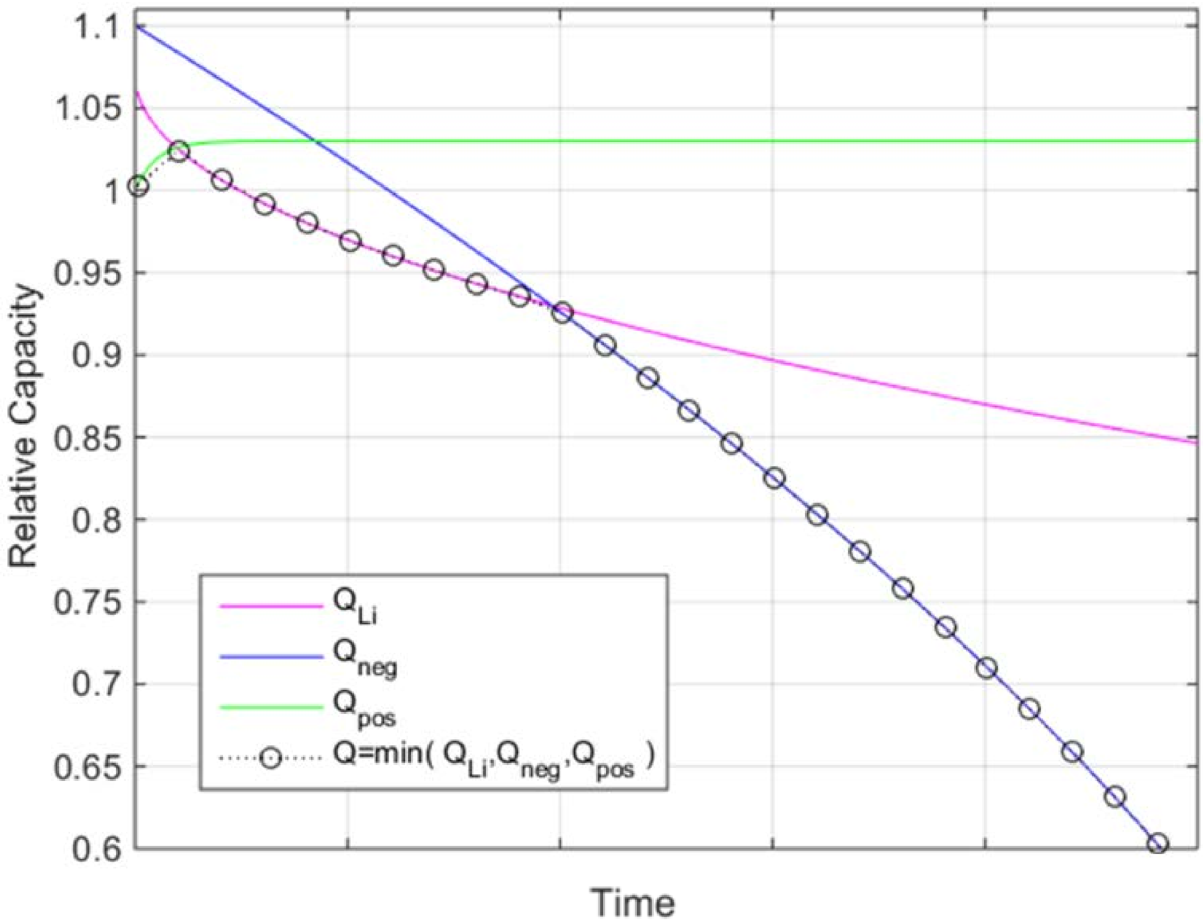
Mechanism	Trajectory equation	State equation	Parameters
Diffusion-controlled reaction	$x(t)=kt^{1/2}$	$\dot{x}(t)=\frac{k}{2}\left(\frac{k}{x(t)}\right)$	*k – rate (p=1/2)*
Kinetic-controlled reaction	$x(t)=kt$	$\dot{x}(t)=k$	*k – rate (p=1)*
Mixed diffusion/kinetic	$x(t)=kt^p$	$\dot{x}(t)=kp\left(\frac{k}{x(t)}\right)^{\left(\frac{1-p}{p}\right)}$	*k – rate, p – order, $0.3<p<1$*
Diffusion controlled reaction with mechanical damage	See Appendix A	$\dot{D}=\frac{dN}{dt}k_D\cdot\left(\sqrt{D}\right)^p$ $\dot{x}_0(t)=\frac{k}{2}\left(\frac{k}{x(t)}\right)$ $\dot{x}_j(t)=D\frac{k}{2}\left(\frac{k}{x(t)}\right)$	*k – rate, p – order*
Cyclic fade – linear	$x(N)=kN$	$\dot{x}(N)=k$	*k – rate (p=0)*
Cyclic fade – accelerating	$x(N)=\left[x_0^{1+p}+kx_0^{\ p}(1+p)N\right]^{\frac{1}{1+p}}$	$\dot{x}(N)=k\left(\frac{x_0}{x(N)}\right)^p$	*k – rate, p – order, $0\geq p>3$*
Break-in process	$x(t)=M(1-\exp(-kt))$ or $x(N)=\ldots$	$\dot{x}(t)=k(M-x(t))$	*M – maximum fade, k – rate*
Sigmoidal reaction	$x(t)=M\left[1-\frac{2}{1+\exp(kt^p)}\right]$ or $x(N)=\ldots$	$\dot{x}(t)=\frac{2MkpX(t)\exp(kX(t))}{[1+\exp(kX(t))]^2}$ $X(t)=\left\{\frac{1}{k}\ln\left(\frac{2}{1-x(t)/M}-1\right)\right\}^{\frac{1}{p}}$	*M – maximum fade, k – rate, p – order*

x, D: state variables
k, k_D: fade rates
p: order
M: maximum extent of fade

S. Santhanagopalan, **K. Smith**, J. Neubauer, G.-H. Kim, A. Pesaran, M. Keyser, Design and Analysis of Large Lithium-Ion Battery Systems, Artech House, 2015.

Model assumes measured capacity is minimum of:

1. Cycleable lithium, Q_{Li}
2. Negative electrode sites, Q_{neg}
3. Positive electrode sites, Q_{pos}



Aging tests – Kokam 75Ah Gr/NMC Li-ion cells

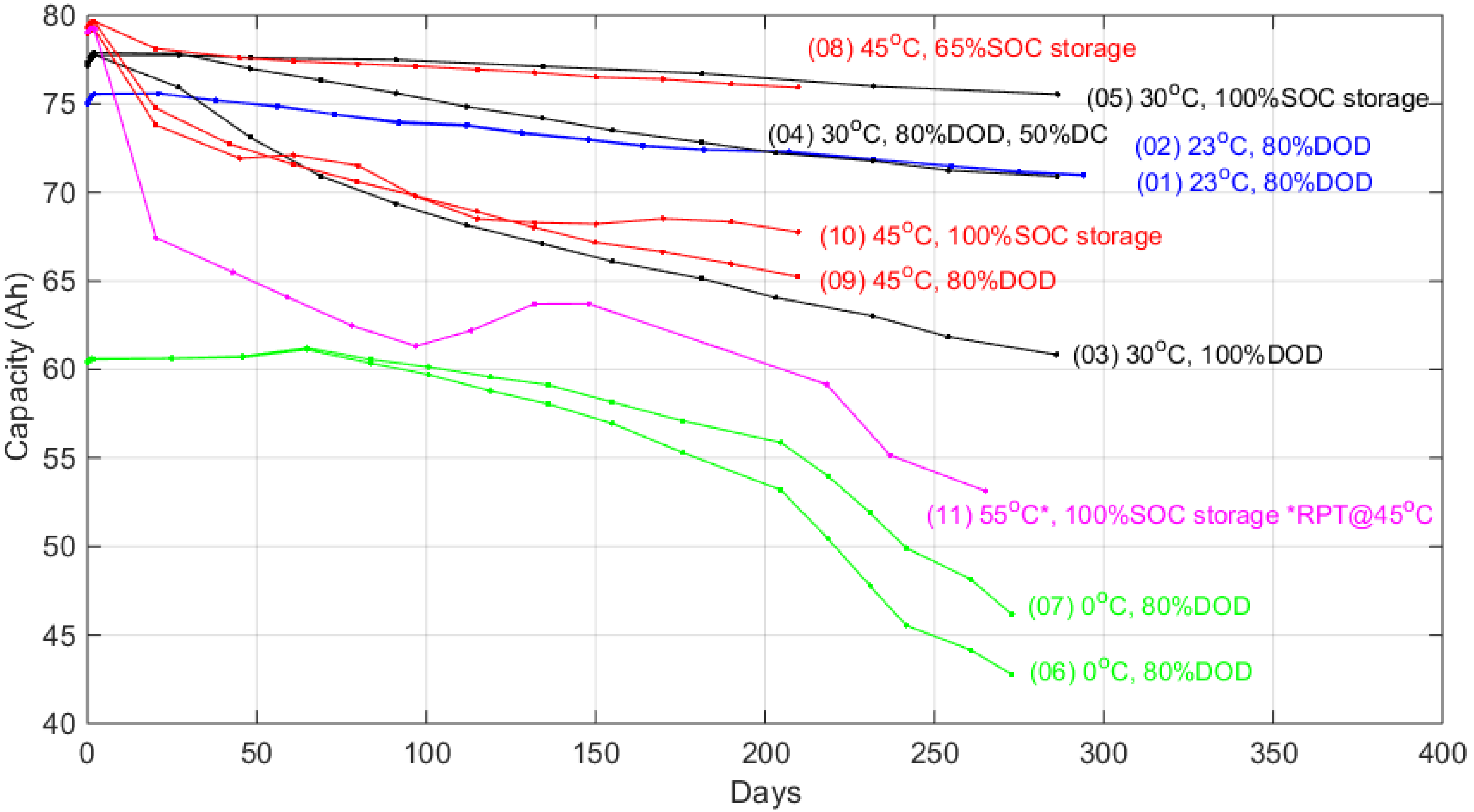
- **Tests design to include both benign and highly accelerated aging**
  - Some real-world, some reaching 30% capacity fade in 6-9 months
- **Pure storage (0%), partial cycling (50% DC*), & fully accelerated cycling (100% DC)**
  - Separate calendar from cycling fade
- **Capacity check run at test temperature**
  - Simplifies testing but makes model ID more difficult
- **Ideal test matrix would include more aging conditions**

Cycling tests				
Temperature	DOD	Dis./charge rate	Duty-cycle*	# of cells
23°C	80%	1C/1C	100%	2
30°C	100%	1C/1C	100%	1
30°C	80%	1C/1C	50%	1
0°C	80%	1C/0.3C	100%	2
45°C	80%	1C/1C	100%	1
Storage tests				
Temperature	SOC			# of cells
30°C	100%			1
45°C	65%			1
45°C	100%			1
55°C	100%			1

Gr = Graphite negative electrode
NMC = Nickel-Manganese-Cobalt positive electrode

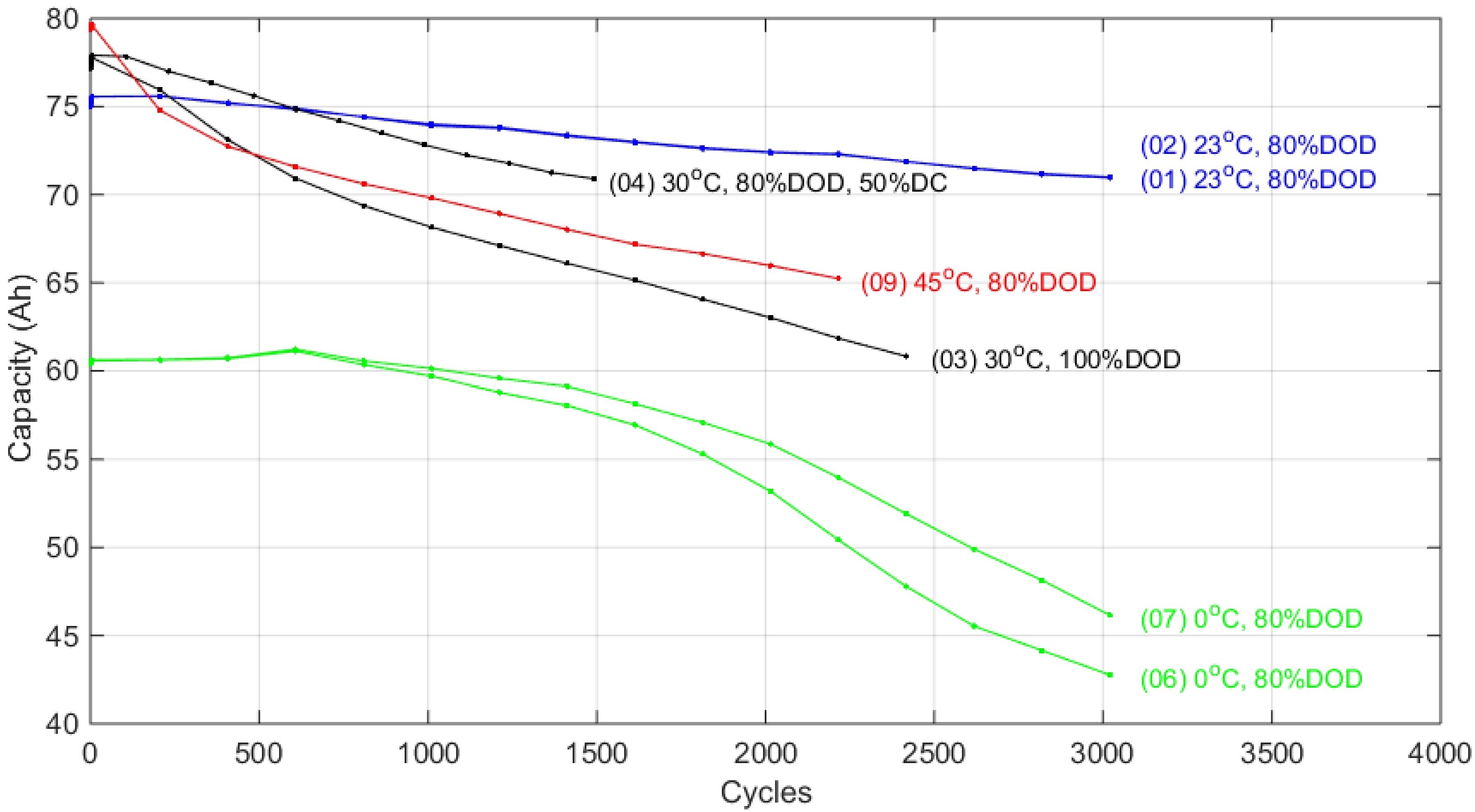
C/5 Capacity vs. Time

- Tight agreement for replicate cells 1&2 at 23°C
- Some divergence for replicate cells 6&7 at 0°C
- Unexplained temporary capacity increase for 55°C storage cell

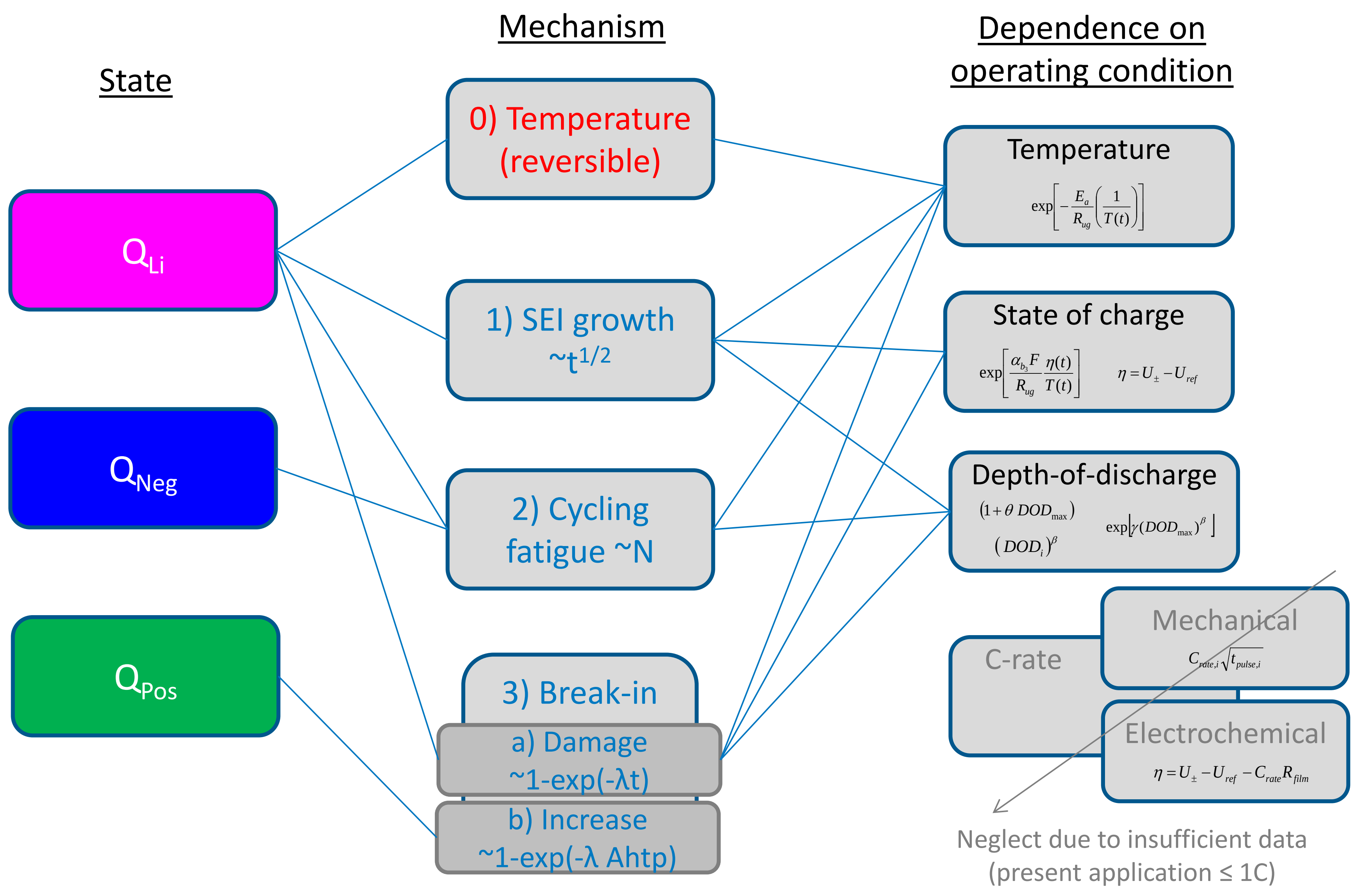


C/5 Capacity vs. Cycles

- **Storage data omitted**
- **Just 6% capacity loss after 3000 cycles at 23°C, 80% DOD**

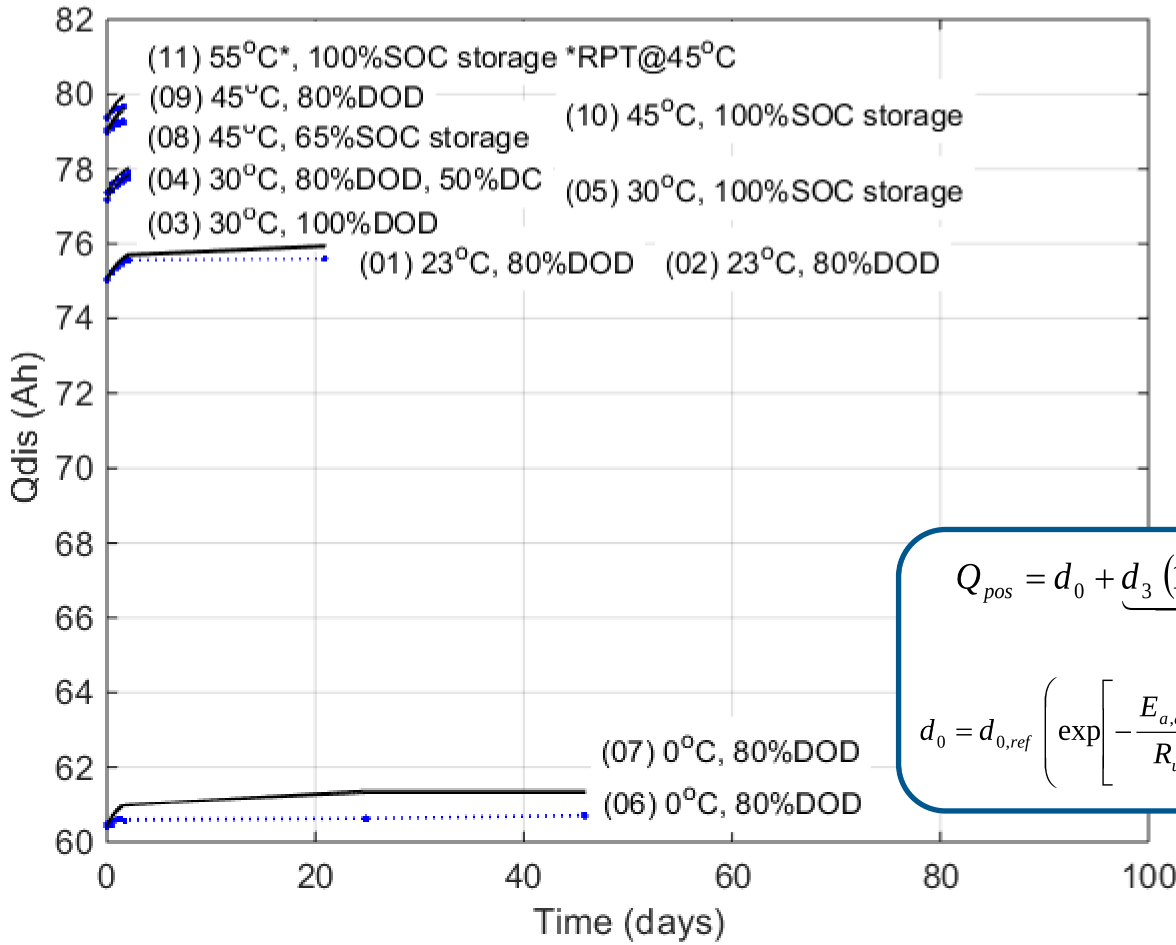


Capacity Evolution–Reversible and Irreversible



Q_{Pos} Capacity Break-in & Initial Temperature Dependence

- **Hypothesize initial cycles induce microcracks in NMC particles, increasing electrolyte wetting and surface area**



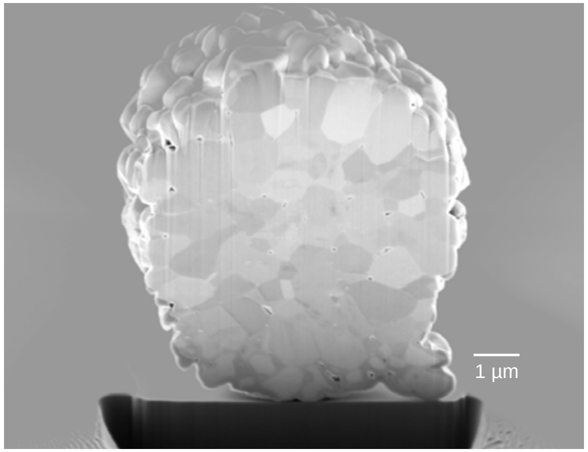


Image: Dean Miller & Daniel Abraham, Argonne National Laboratory

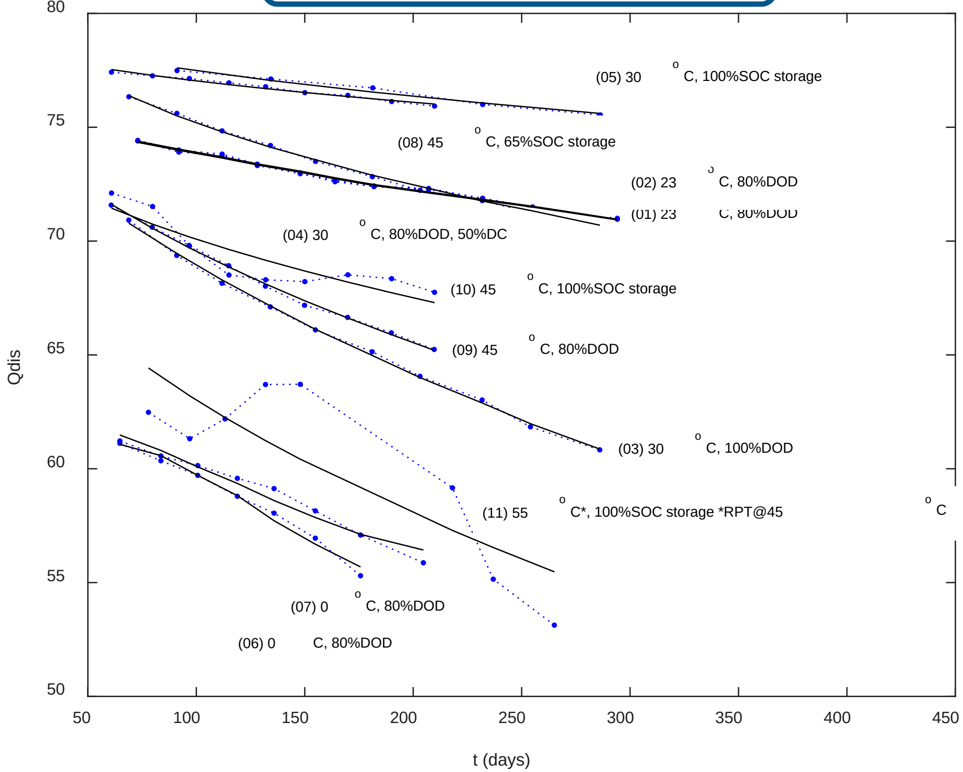
$$Q_{pos} = d_0 + \underbrace{d_3\left(1-\exp(-Ah_{dis}/228)\right)}_{\textit{Increase in capacity at BOL}}$$

$$d_0 = d_{0,ref}\left(\exp\left[-\frac{E_{a,d_0,1}}{R_{ug}}\left(\frac{1}{T_{RPT}(t)}-\frac{1}{T_{ref}}\right) - \left(\frac{E_{a,d_0,2}}{R_{ug}}\right)^2\left(\frac{1}{T_{RPT}(t)}-\frac{1}{T_{ref}}\right)^2\right]\right)$$

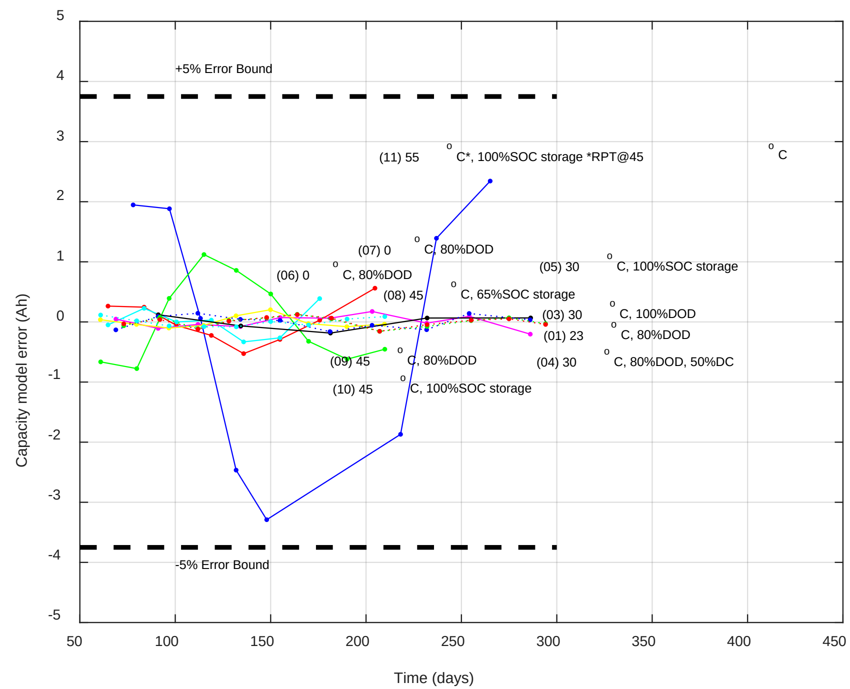
Q_{Li} Local Models

- **Local models: Separately fit b_0, b_1, b_2 for each data set, excluding**
  - o First 50 days of data (allows y-intercept to vary with break-in)
  - o Knee at 0°C (to be captured later with Q_{neg} model)

$$Q_{Li} = d_0 \left[b_0 - b_1 t^{1/2} - b_2 N \right]$$



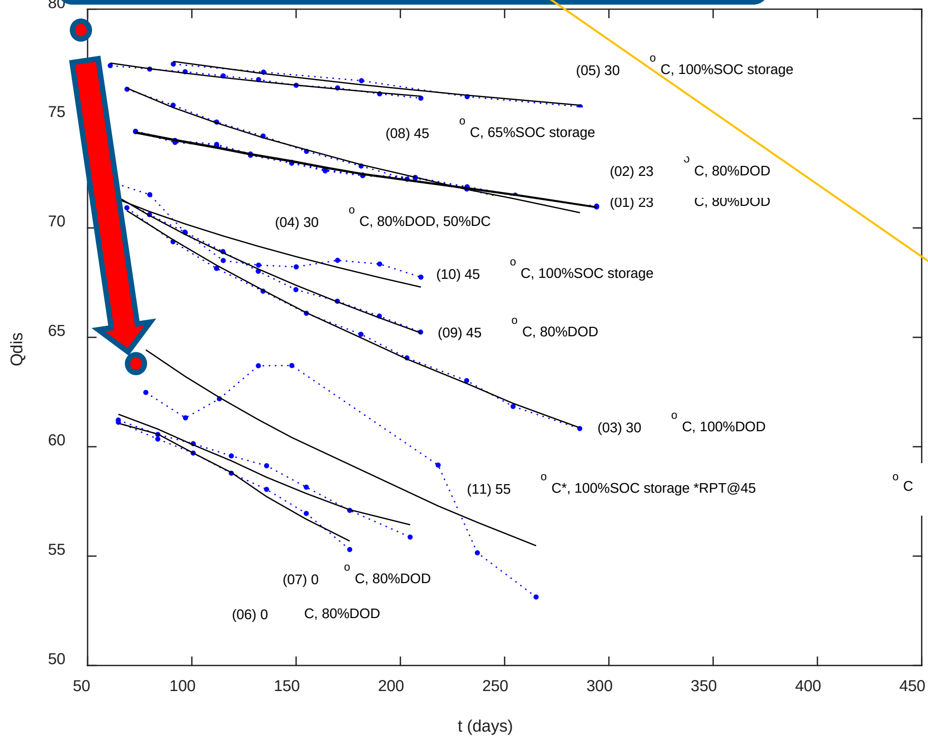
Error = Model - Data



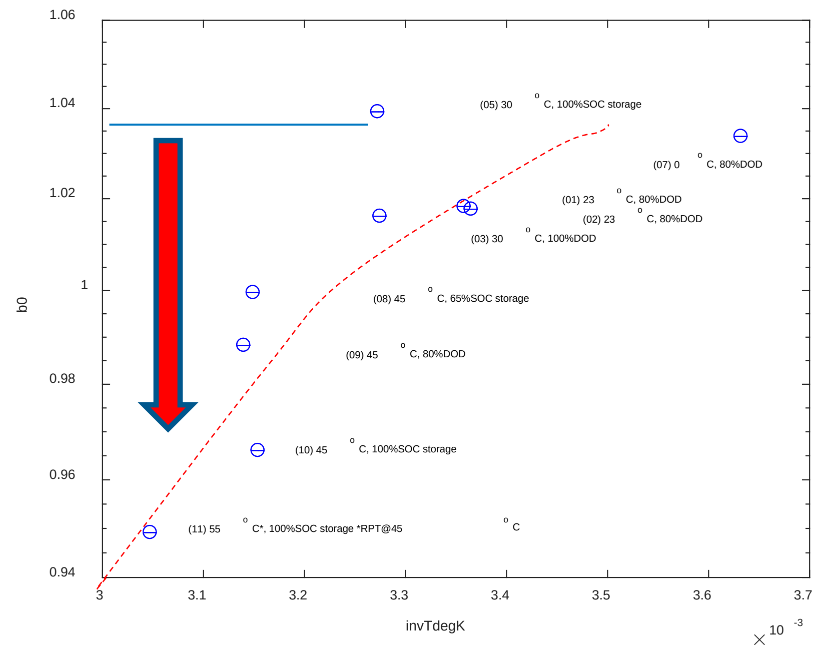
- Choice of mechanisms justified by R^2=0.990 and flat residuals

Q_{Li} Magnitude of break-in Li-loss

Local model $Q_{Li} = d_0\left[b_0 - b_1 t^{1/2} - b_2 N\right]$



b_0 magnitude



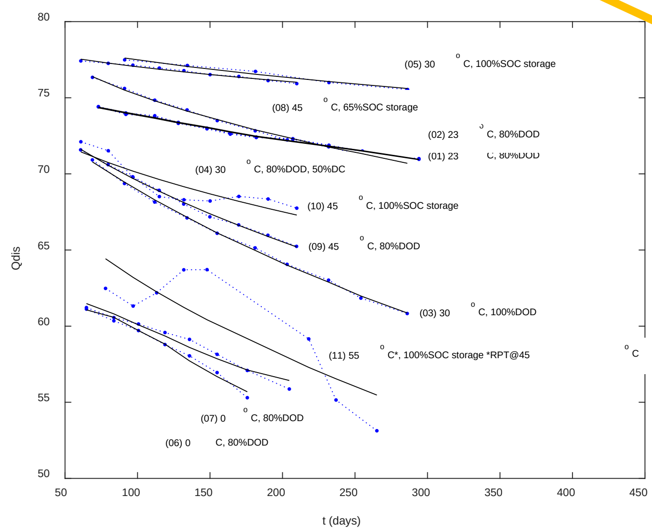
- **Least degraded cells show ~3-4% excess Li capacity**
- **High temperature causes rapid loss in first 50 days**
  - Open-circuit voltage and DOD also increase loss
  - Evidence of film layer formation at positive electrode?

b_0 magnitude model $y_0 - b_3\left(1-\exp(-t/\tau_{b3})\right)$

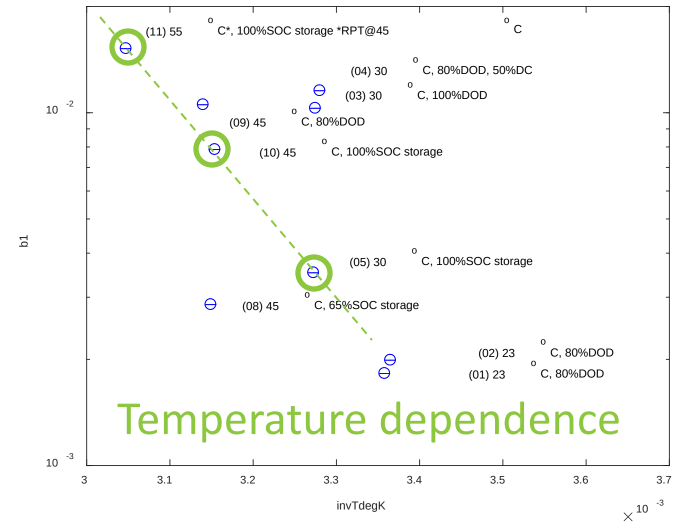
$$b_3 = b_{3,ref}\ \exp\left[-\frac{E_{a,b_3}}{R_{ug}}\left(\frac{1}{T(t)}-\frac{1}{T_{ref}}\right)\right]\ \exp\left[\frac{\alpha_{b_3}F}{R_{ug}}\left(\frac{V_{OC}(t)}{T(t)}-\frac{V_{ref}}{T_{ref}}\right)\right]\ \left(1+\theta\ DOD_{max}\right)$$

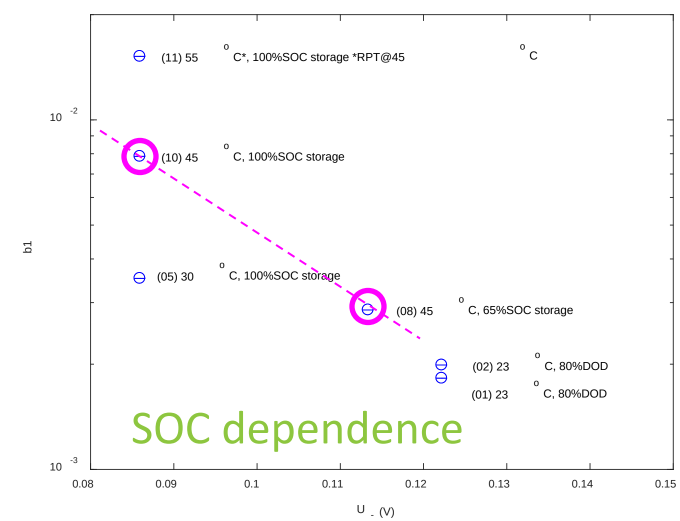
Q_{Li} Calendar fade rate

Local model $Q_{Li} = d_0 \left[b_0 - b_1 t^{1/2} - b_2 N \right]$



b₁ rate





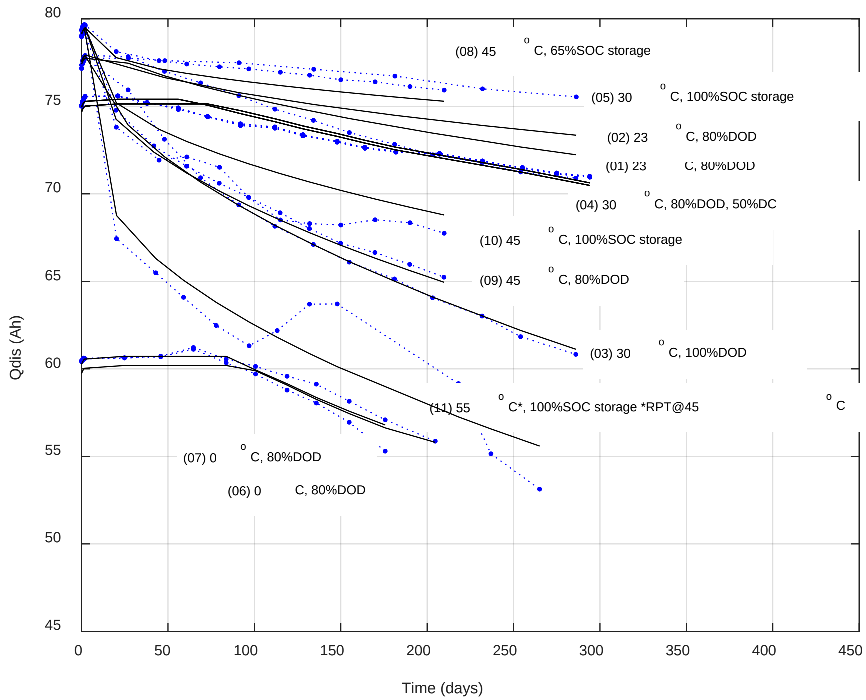
b_1 rate model

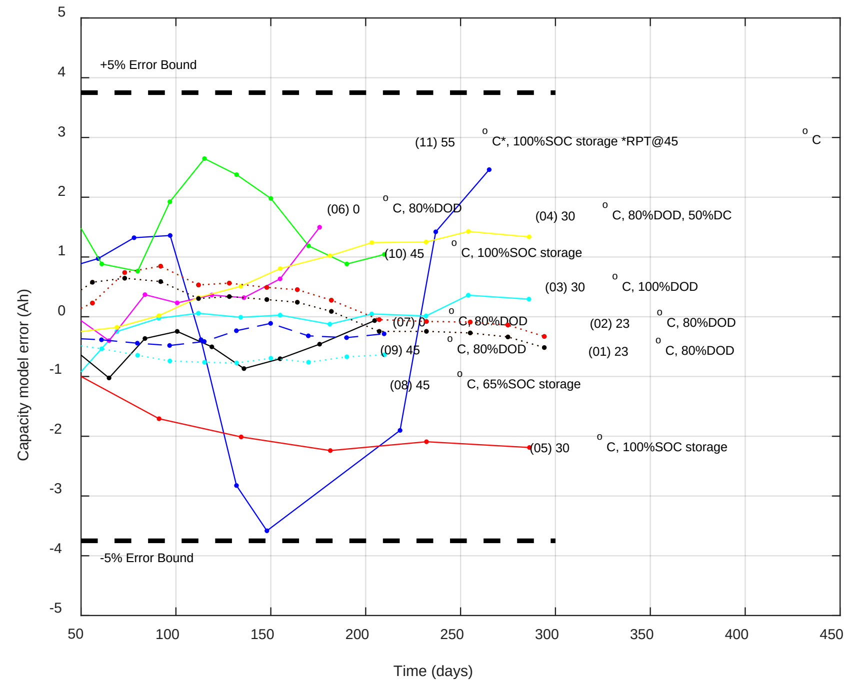
$$b_1 = b_{1,ref} \exp\left[-\frac{E_{a,b_1}}{R_{ug}} \left(\frac{1}{T(t)} - \frac{1}{T_{ref}} \right) \right] \exp\left[\frac{\alpha_{b_1} F}{R_{ug}} \left(\frac{U_-(t)}{T(t)} - \frac{U_{ref}}{T_{ref}} \right) \right] \exp\left[\gamma_{b_1} (DOD_{max})^{\beta_{b1}} \right]$$

- **Visualization of rates suggests rate model equations**
- **Fitted rate model parameters provide initial guess for global model parameters**

Q_{Li} Global Model

- **With equations known, parameters fit to all data simultaneously**
- **R^2 = 0.985, RMSE = 1% of capacity, flat residuals**





Q_{Li} global model

$$Q_{Li} = d_0 \left[b_0 - \underbrace{b_1 t^{1/2}}_{\text{SEI growth with calendar time}} - \underbrace{b_2 N}_{\text{Loss with cycling}} - \underbrace{b_3\left(1-\exp(-t/\tau_{b3})\right)}_{\text{Break-in mechanism at BOL}} \right]$$

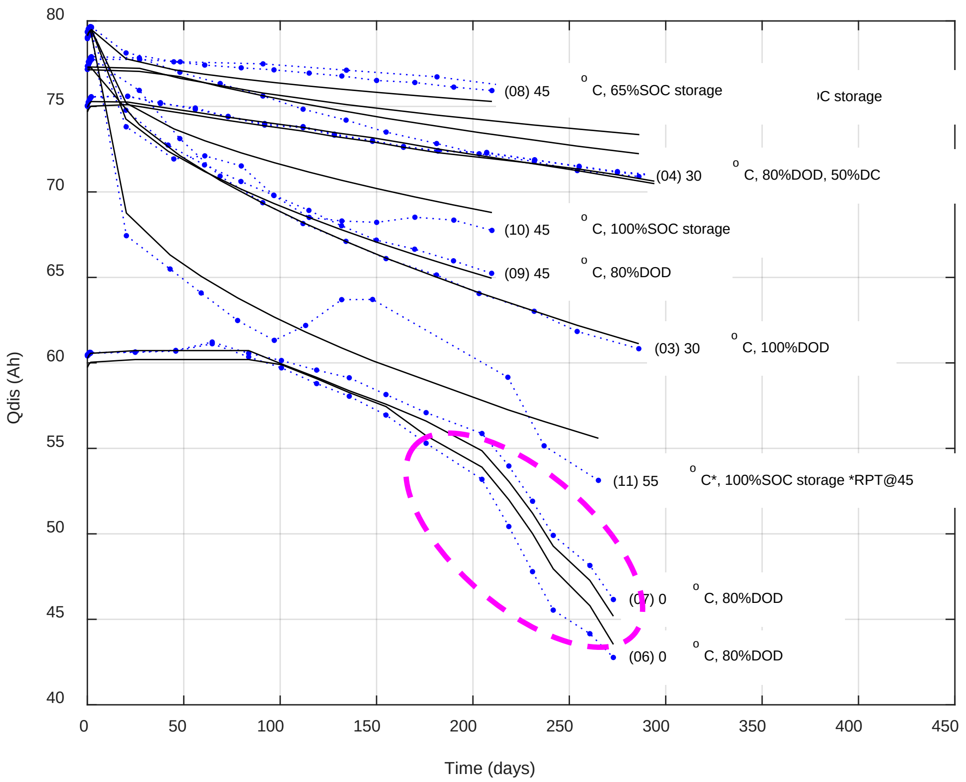
$$b_1 = b_{1,ref}\ \exp\left[-\frac{E_{a,b_1}}{R_{ug}}\left(\frac{1}{T(t)}-\frac{1}{T_{ref}}\right)\right]\ \exp\left[\frac{\alpha_{b_1}F}{R_{ug}}\left(\frac{U\_(t)}{T(t)}-\frac{U_{ref}}{T_{ref}}\right)\right]\ \exp\left[\gamma_{b_1}(DOD_{\max})^{\beta_{b1}}\right]$$

$$b_2 = b_{2,ref}\ \exp\left[-\frac{E_{a,b_2}}{R_{ug}}\left(\frac{1}{T(t)}-\frac{1}{T_{ref}}\right)\right]$$

$$b_3 = b_{3,ref}\ \exp\left[-\frac{E_{a,b_3}}{R_{ug}}\left(\frac{1}{T(t)}-\frac{1}{T_{ref}}\right)\right]\ \exp\left[\frac{\alpha_{b_3}F}{R_{ug}}\left(\frac{V_{OC}(t)}{T(t)}-\frac{V_{ref}}{T_{ref}}\right)\right]\ \left(1+\theta\ DOD_{\max}\right)$$

Q_{Neg} Model

- Captures **knee** with cold temperature cycling
- Minor importance in most real-world scenarios



Q_{Neg} global model

$$\frac{dQ_{neg}}{dN} = -\left(\frac{c_2}{Q_{neg}}\right)$$

$$Q_{neg} = \left[c_0{}^2 - 2c_2c_0\ N\right]^{\frac{1}{2}}$$

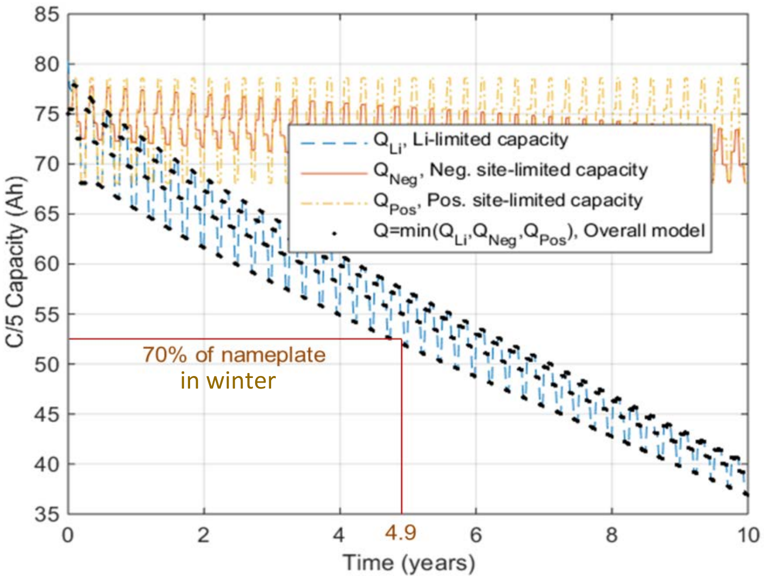
$$c_0 = c_{0,ref}\ \exp\left[-\frac{E_{a,c0}}{R_{ug}}\left(\frac{1}{T(t)} - \frac{1}{T_{ref}}\right)\right]$$

$$c_2 = c_{2,ref}\ \exp\left[-\frac{E_{a,c_2}}{R_{ug}}\left(\frac{1}{T(t)} - \frac{1}{T_{ref}}\right)\right](DOD)^{\beta_{c2}}$$

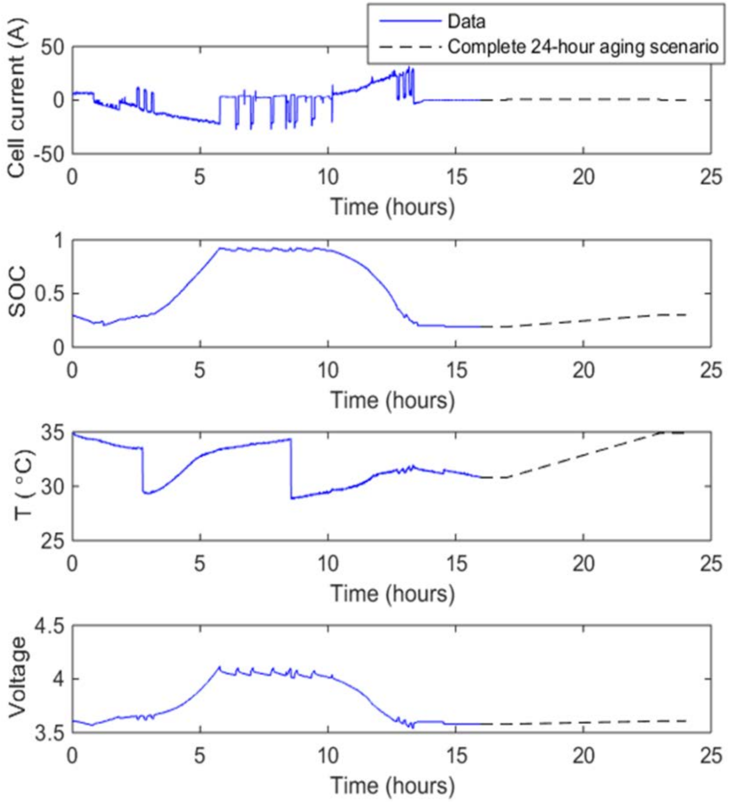
Lifetime analysis – PV self consumption

- **Model reformulated in rate-based form**
- **SOC(t) discretized into microcycles, DOD_i, using Rainflow algorithm**

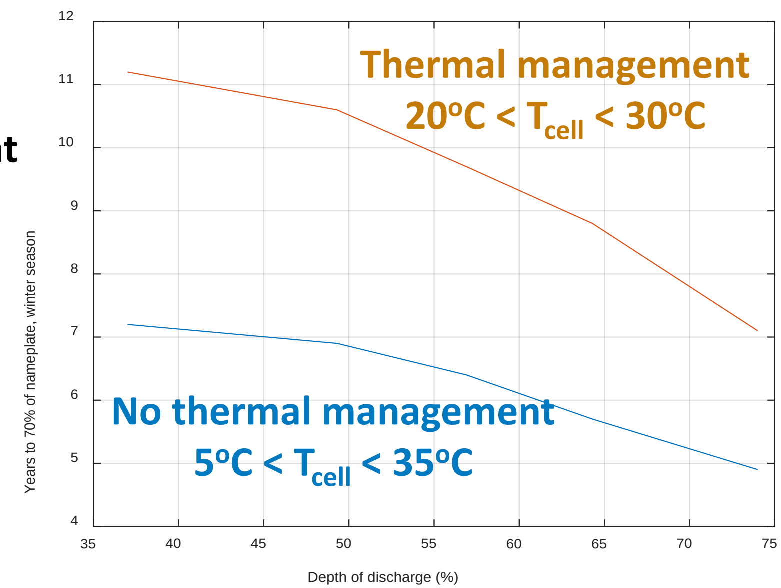
- **Multi-year, 4-season simulation**
- **Same cycle each**



- **Application data**



- **Impact of DOD and thermal management**



Conclusions

- **Battery energy storage can enable increased integration of renewable power generation on the grid**
- **Battery life modeling methodology formalized, aiding systems design process**
  - Capacity error: $L_2 = 1\%$, $L_\infty = 5\%$
  - For studied Gr/NMC Li-ion ES technology, best to restrict daily cycles < 55% DOD with occasional larger excursions
  - Thermal management extends life from 7 to 10 years
- **Battery aging experiments are time consuming & expensive**
- **Additional model validation needed**
  - Longer duration
  - Variable cycling & temperature
- **Life model accuracy may be enhanced in the future by coupling with electrochemical modeling & diagnostics**

Acknowledgements

- U.S. DOE Office of Energy Efficiency and Renewable Energy Solar Energy Technologies Program
- SunPower Corporation

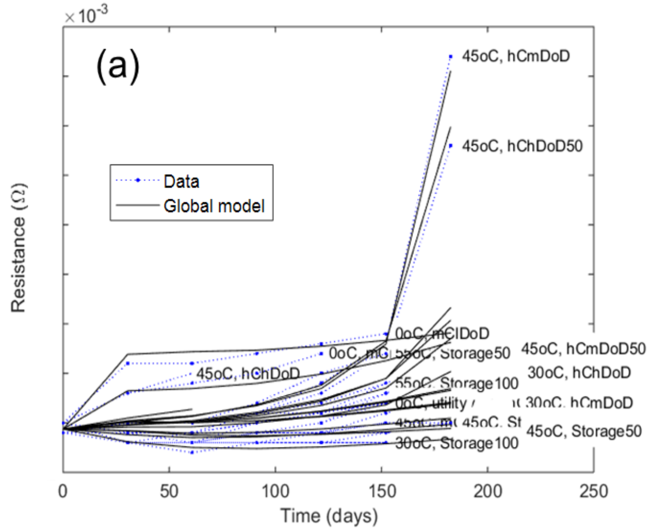
Extra Slides

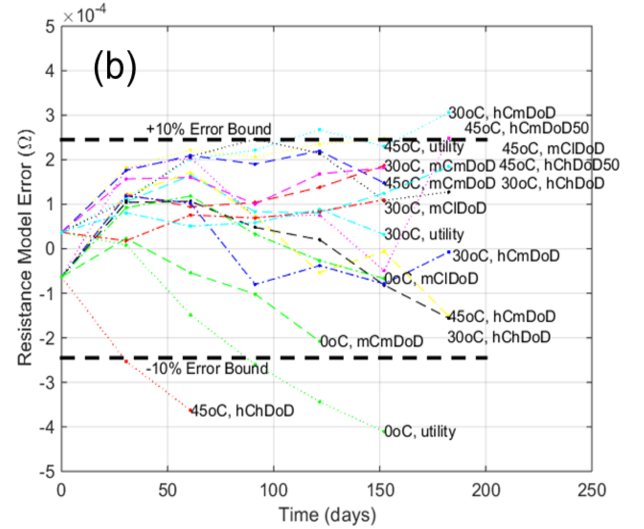
Previous Validation of Life Model

Eaton Corp. ARPA-E AMPED project resulting in 35% smaller HEV battery (PI: Dr. Chinmaya Patil/Eaton)

Cell-level aging tests

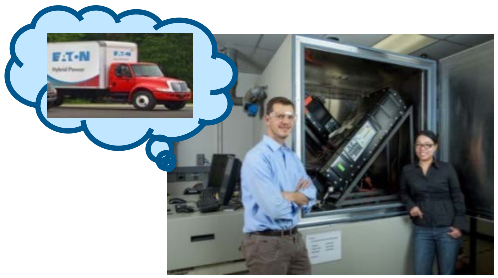
Prognostic model characterization

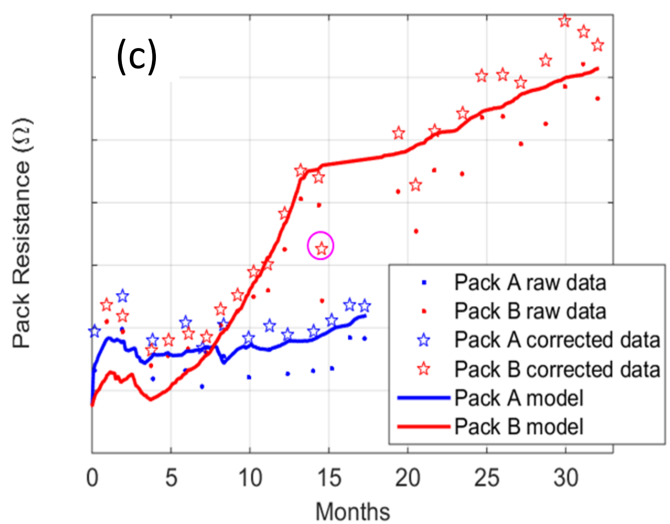


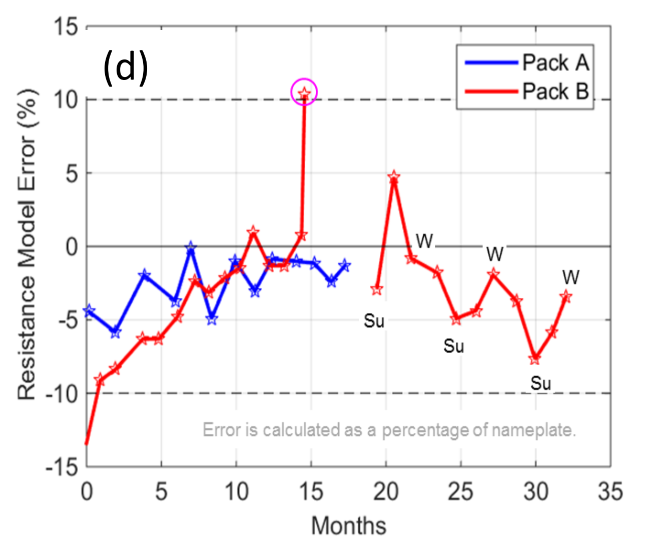


Pack-level HIL tests

HEV prognostic control algorithm validation







Model tuned to 6 months simple cell aging data matches 33 months 4-season cycling with same accuracy