Physics-Informed ROM Development for ISS EMU LLB-2 Condition-Based Monitoring

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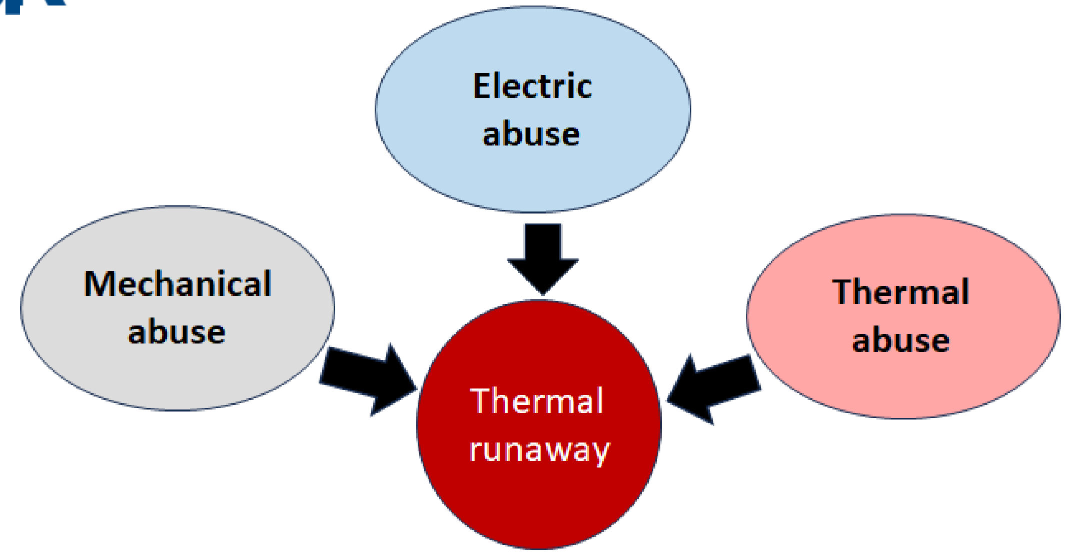
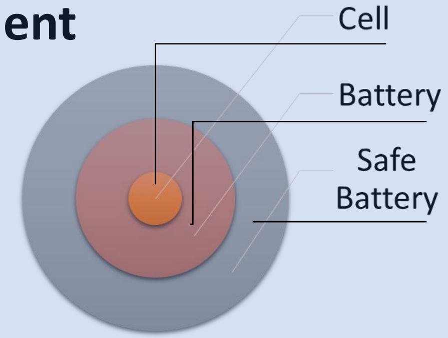
Need for Anomaly Detection



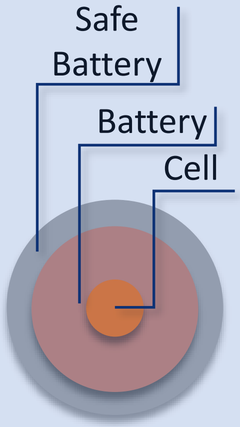
- Mechanical abuse: deformation, crash
- Electric abuse: over-charging, over-discharging
- Thermal abuse: overheating

- SOA approach: containment



Alternative

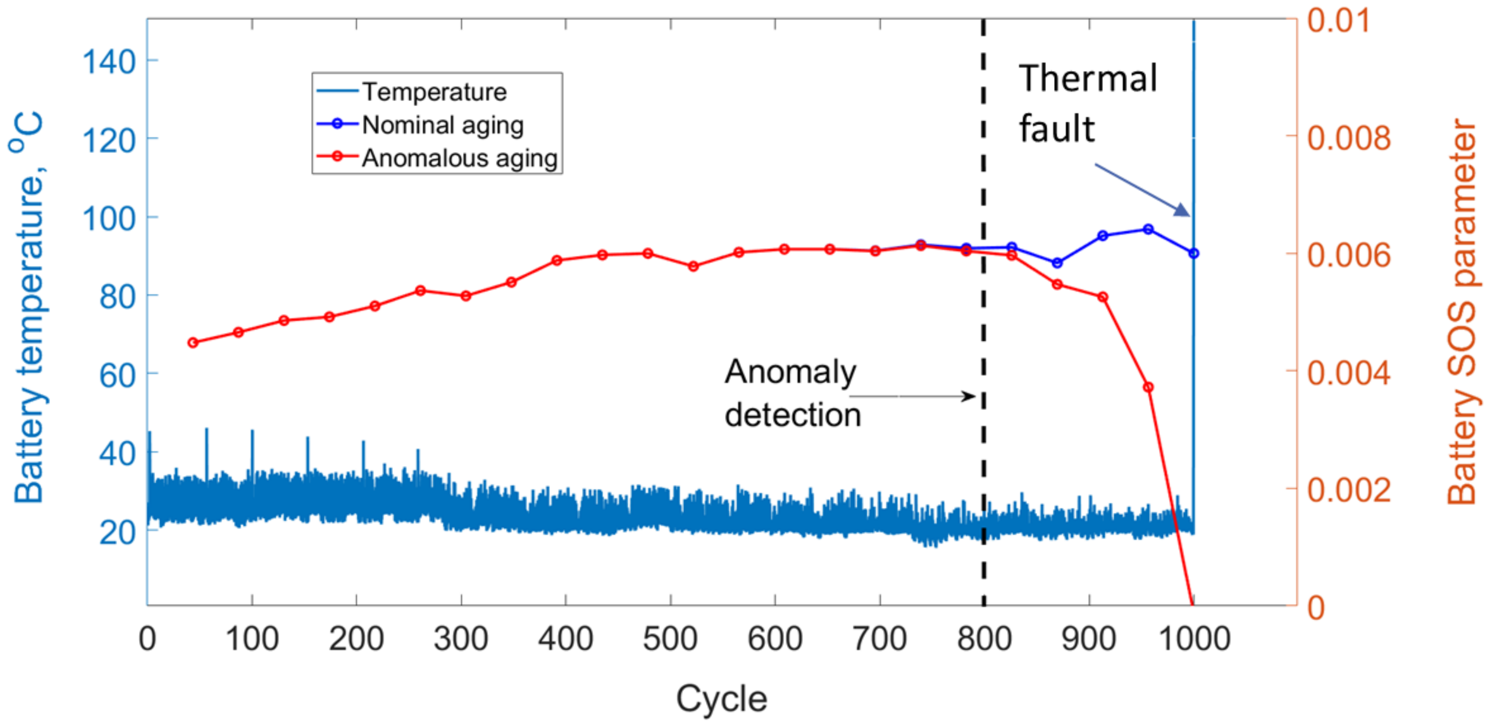
Smart BMS:
- ✓ In-situ sensors
- ✓ Predictive framework



- Cons: Weight Penalty for Safety
- Smart BMS: reduction of the battery weight

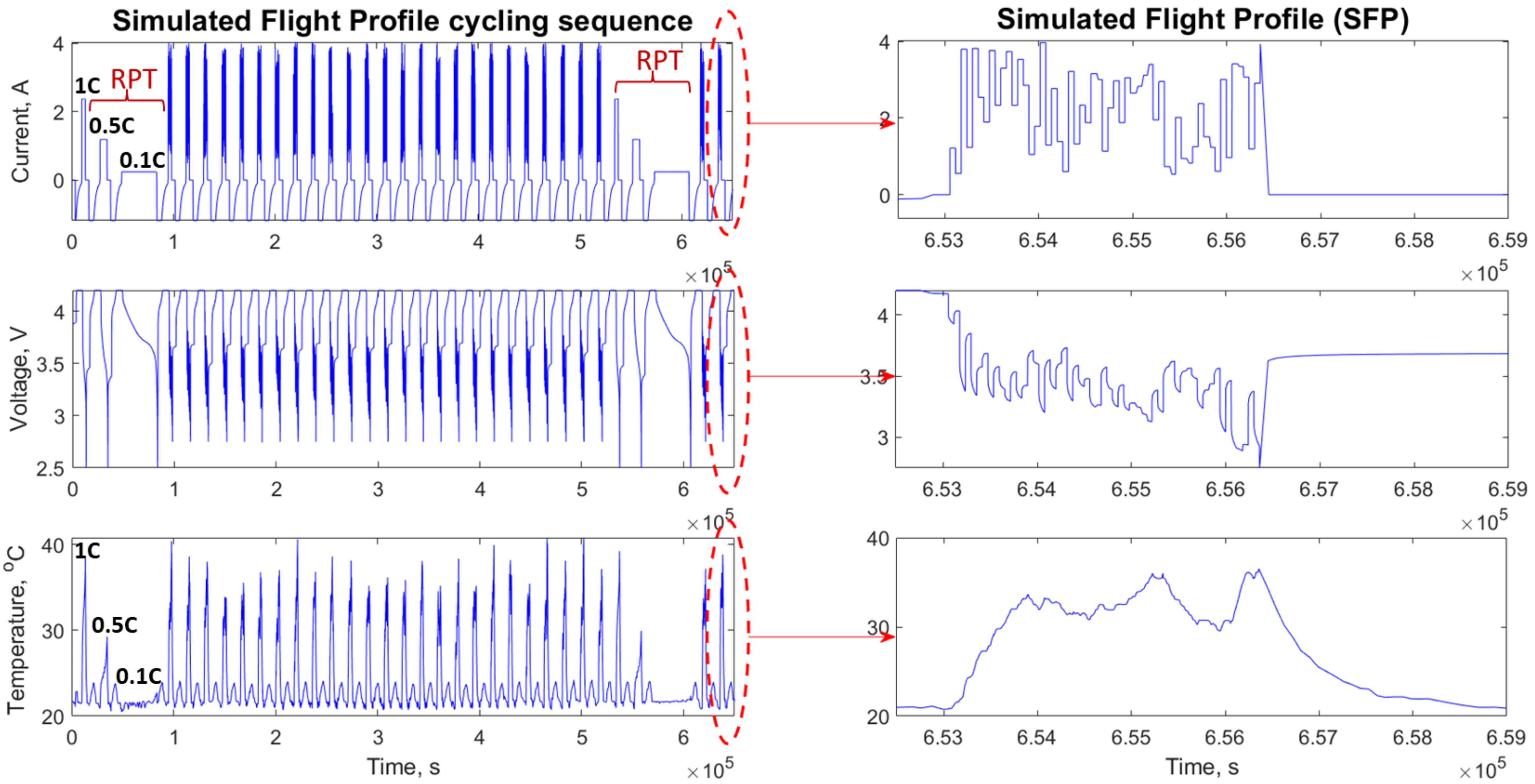
Anomaly detection from field data

Schematics of an anomaly detection from thermal data



- Anomalies can reflect faults which can become catastrophic over time
- SOA BMS track anomalies in few parameters: capacity, internal resistance and typical maximal temperature
- Field (flight) data contains more information
- **Retrieving this information is challenging**

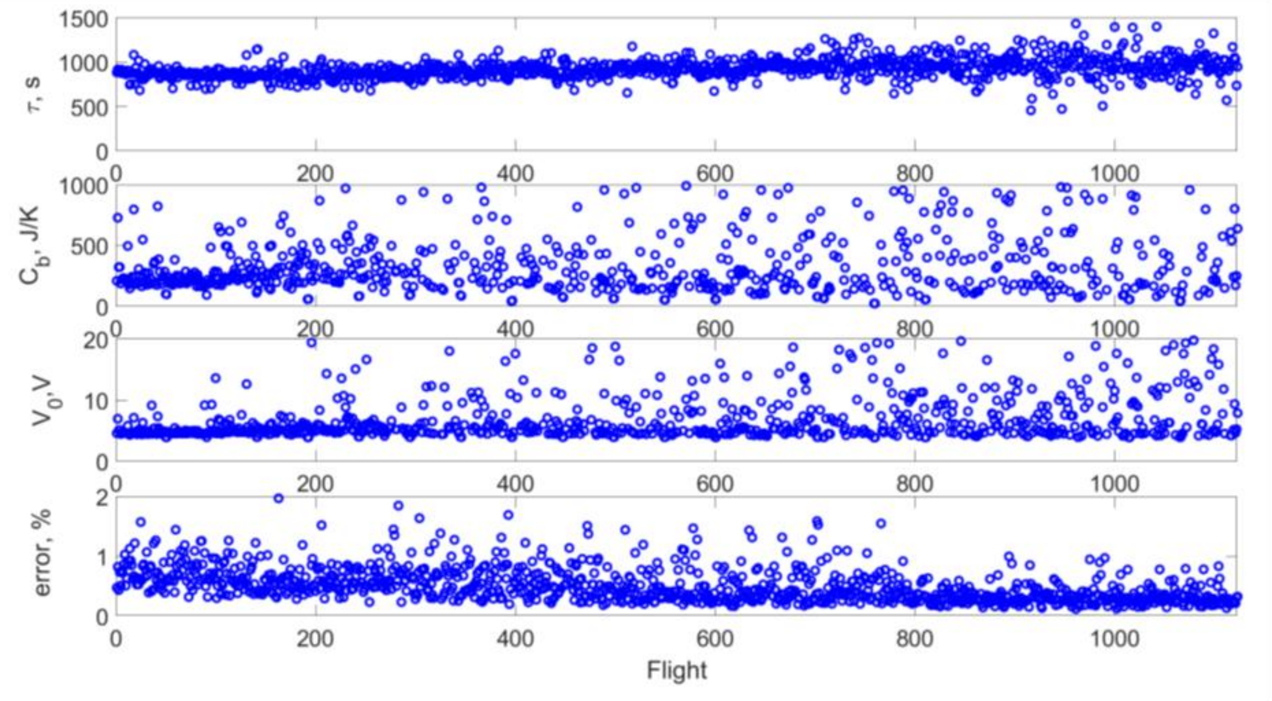
Testing protocol: RPT + SFP



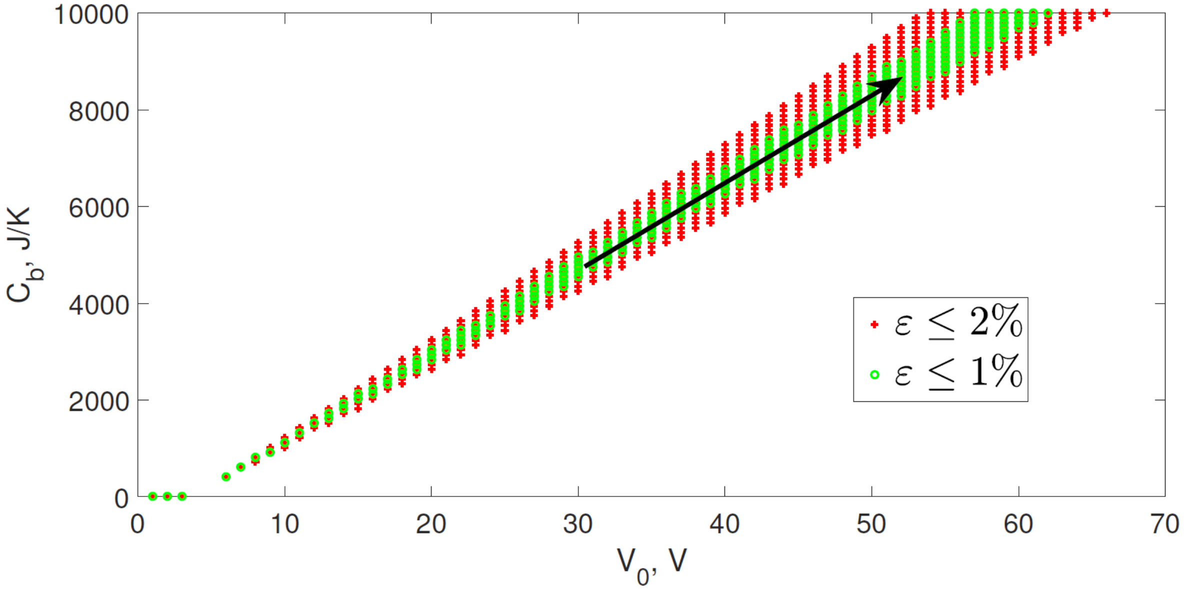
A need for Identifiable models

3pTROM:

$$T = T_a + [T(0) - T_a]e^{-t/\tau} + C_b^{-1}\int_0^t I(t')[V_0 - V(t')]e^{\frac{t'-t}{\tau}}dt' ,$$



Non-identifiable.



The underlying reason: quasi-degeneracy of the RMSE landscape in the parameter space.

The landscape suggests the model reduction path (black arrow)

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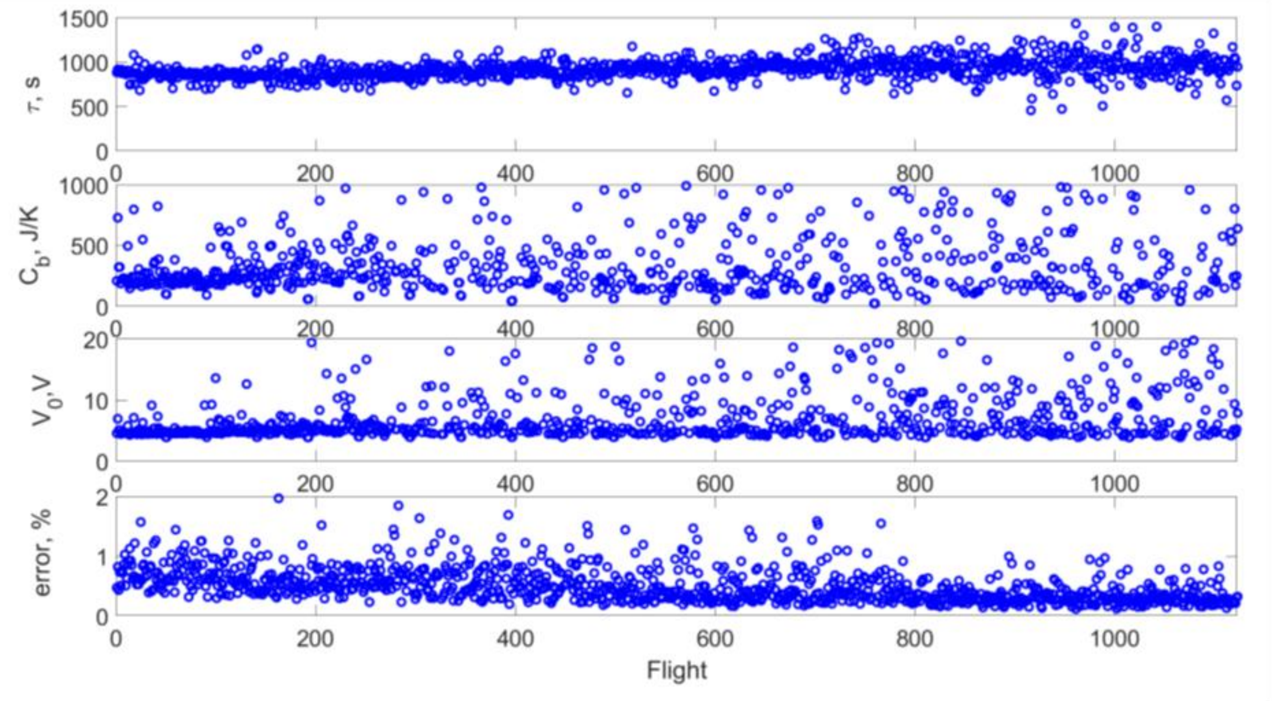
Model reduction leads to identifiability

3pTROM:

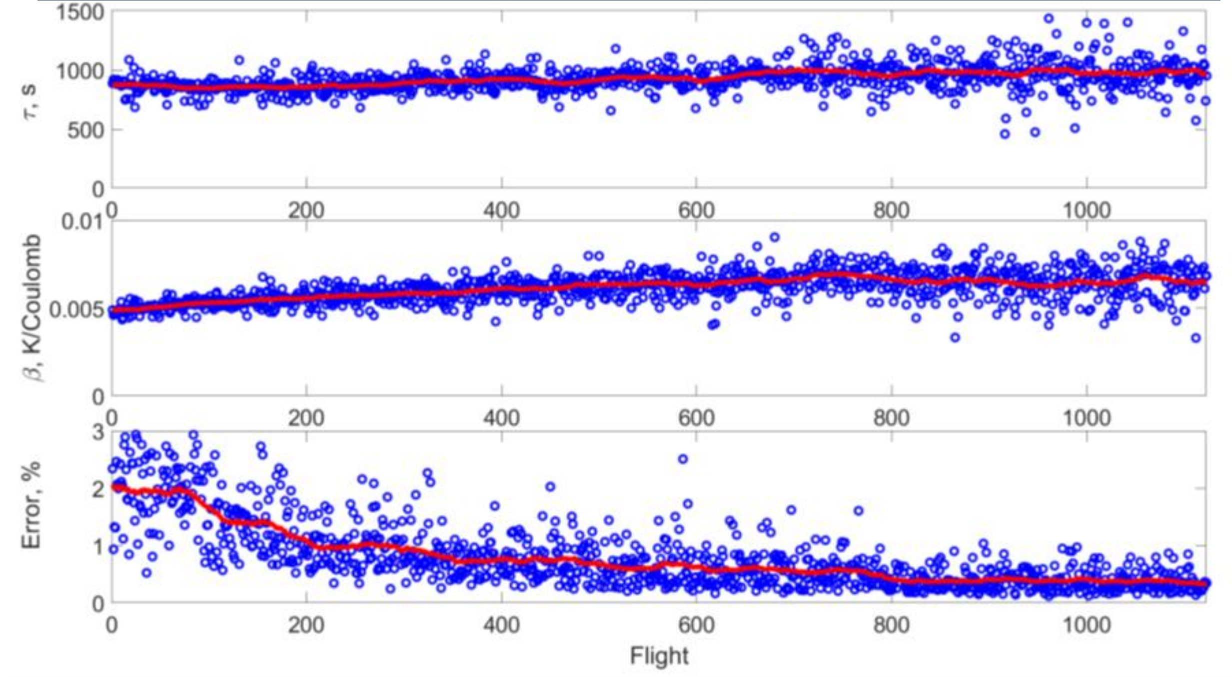
$$T = T_a + [T(0) - T_a]e^{-t/\tau} + C_b^{-1}\int_0^t I(t')[V_0 - V(t')]e^{\frac{t'-t}{\tau}}dt',$$

2pTROM:

$$T = T_a + [T(0) - T_a]e^{-t/\tau} + \beta\int_0^t I(t')e^{\frac{t'-t}{\tau}}dt'$$



Non-identifiable.



Identifiable

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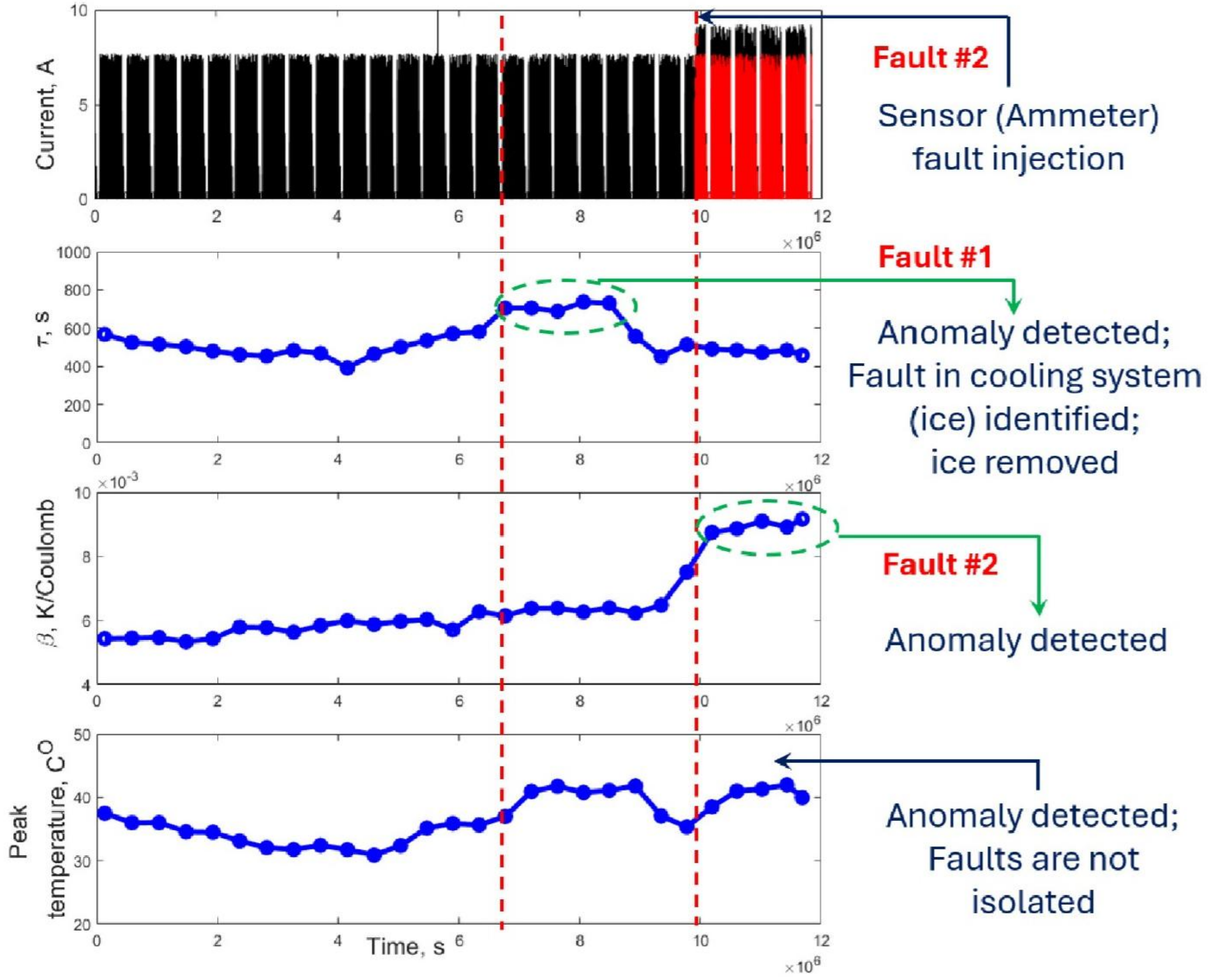
Anomaly detection using 2pTROM



Experimental Context:
- MJ1 (NMC) cell cycled under the RW protocol.
- Validates 2pTROM against Actuator vs. Sensor faults.

Fault 1: Cooling System Failure (Ice Formation)
- Signal: Sharp increase in Cooling Time (**τ**).
- Physics: Ice reduced the convective heat transfer coefficient; β remained invariant.

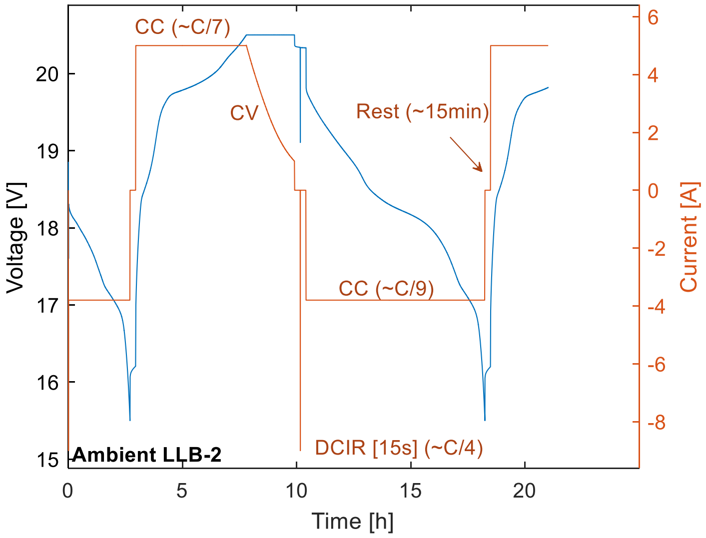
Fault 2: Ammeter Bias (-20% Reporting Error)
- Signal: Step discontinuity in Thermal Susceptibility (β).
- Physics: Model increases β to compensate for under-reported Ohmic heating (~ **β*I**).

Key Result:
- Fault Isolation Ambiguity: Peak temperature ($\mathbf{T_{max}}$) rises in both scenarios.
- Resolution: Parameter orthogonality (**τ** vs. **β**) decouples the failure modes.

Mehta, M. R., Crowley, K. M., Khasin, M., Kulkarni, C. S., DeMattia, B., & Lawson, J. W. (2025). "Anomaly detection in Li-ion cells using physics-based reduced-order thermal models." *Journal of Power Sources*, 631, 236190.

Workflow: from data to prognostics

Data



Challenge: data is limited

Features/health indicators:
e.g., total resistance (R_{eff}) and capacity (Q)

Challenge: features are limited

Diagnostics

and Prognostics

Data Available from ISS EBOT and EMU

- **8 ISS EVAs per year (~45 days between EVAs)**
- **Batteries stored at 30-50% state-of-charge (SoC)**
- **Charged 2 weeks prior to EVA**
- **Charging time of 10 hours**
- **Batteries at 100% SoC for 2 weeks**
- **EVA time of 7 hours**

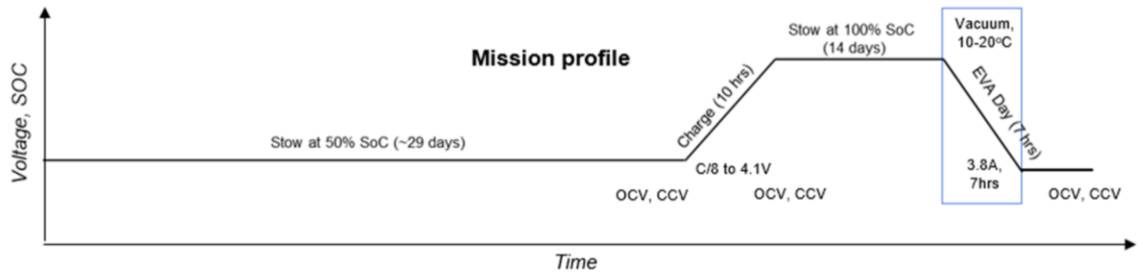
5S Charge Configuration:
- 15.5-20.5Vdc (3.1-4.1Vdc per cell)

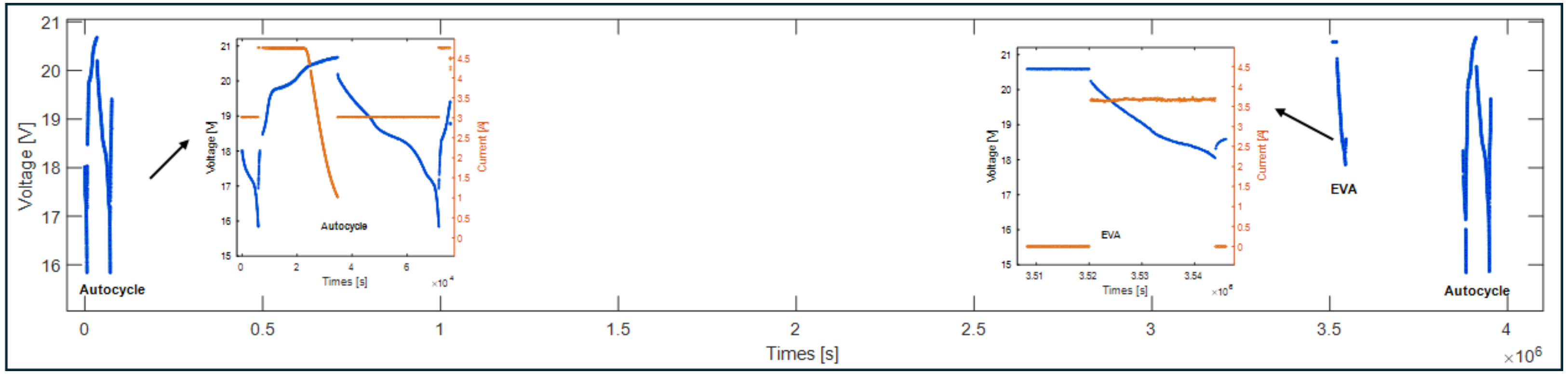
Para	LLB2	LREBA	LPGT
Charge (A)	5	3	2
Discharge (A)	2.5		
8hr EVA (A)	3.8		

Life Limits:
- 600 days over 50%
- 5 years
- 25 cycles (100% DOD)

Non-EVA Env:
- 10-12 psia, 20°C

EVA Env:
- vacuum, 10-20°C

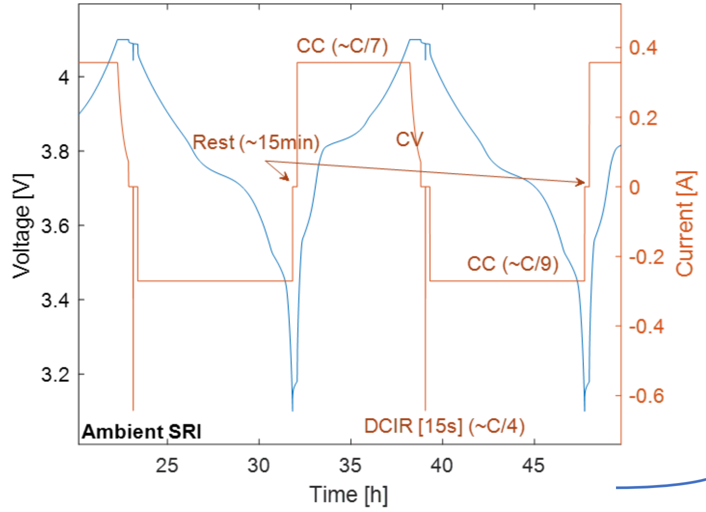




1. Pack-level voltage data (bank voltages not transmitted)
2. Aging shaped mostly by calendar aging

Data Available from Ground Testing Campaign

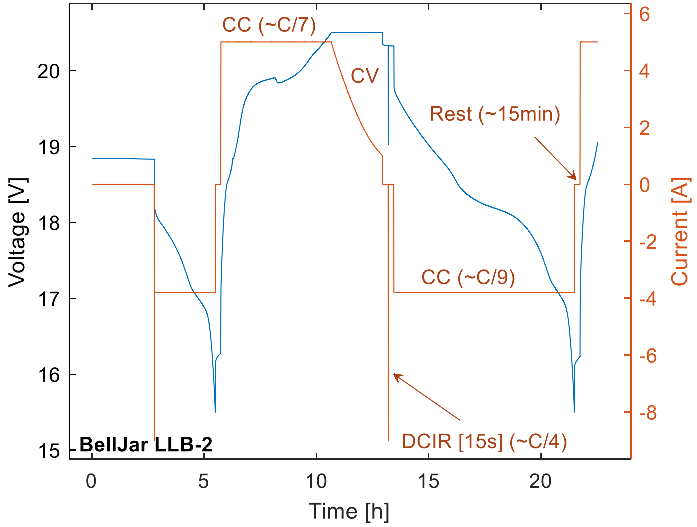
Single Cell Cycling



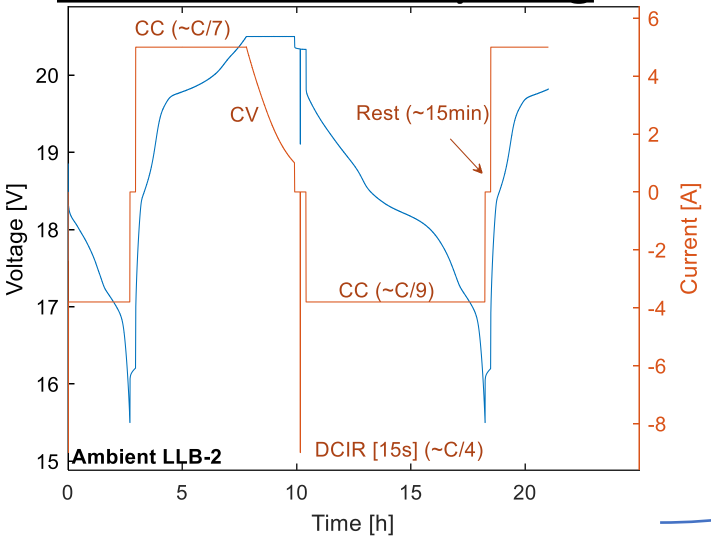
Ambient Cycling of 20 Samsung ICR18650-26F Cells

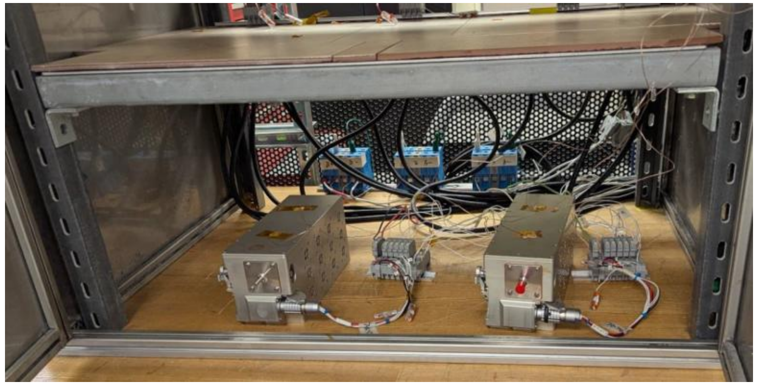
1. Cell level voltage data
2. Aging is shaped by cycling

Bell Jar Pack Cycling



Ambient Pack Cycling





1. Bank level voltage data
2. Temperature data
3. Aging is shaped by cycling

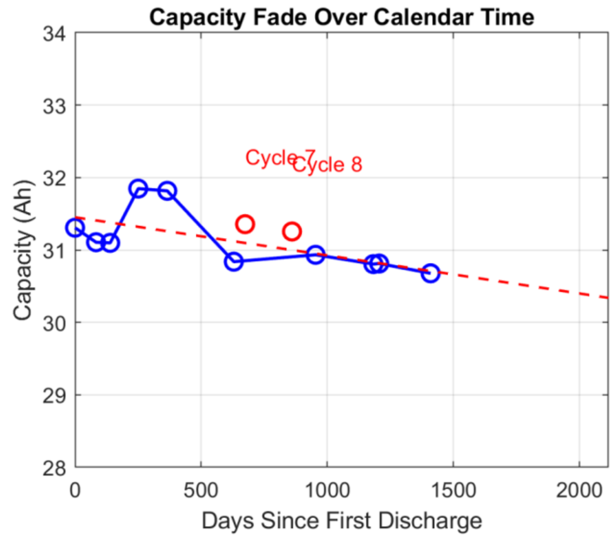
The challenge: data is limited

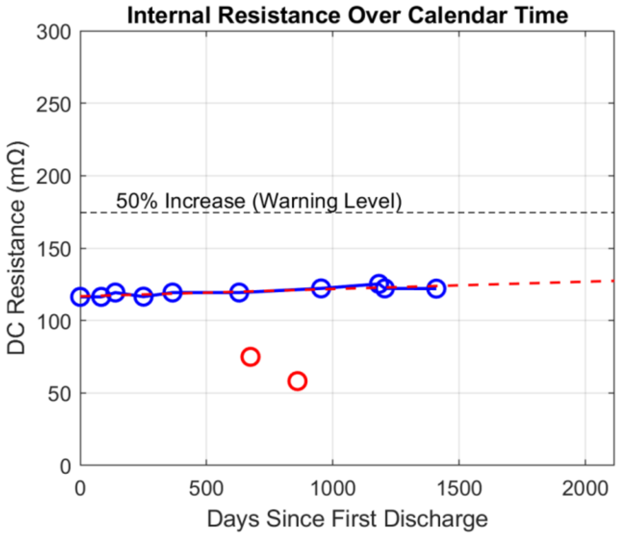
- **Limited data channels/telemetry (ISS data):**
  - ✓Pack-level voltage telemetry (masking effect)
  - ✓Bank voltage and temperature monitored but not transmitted

- **Limited testing regimes (ESTA tests):**
  - ✓Cycling aging is tested
  - ✓Calendar aging is not tested*

* Earlier cell level calendar aging data is available

Conventional analysis: Reff and Q. LLB-2#1005





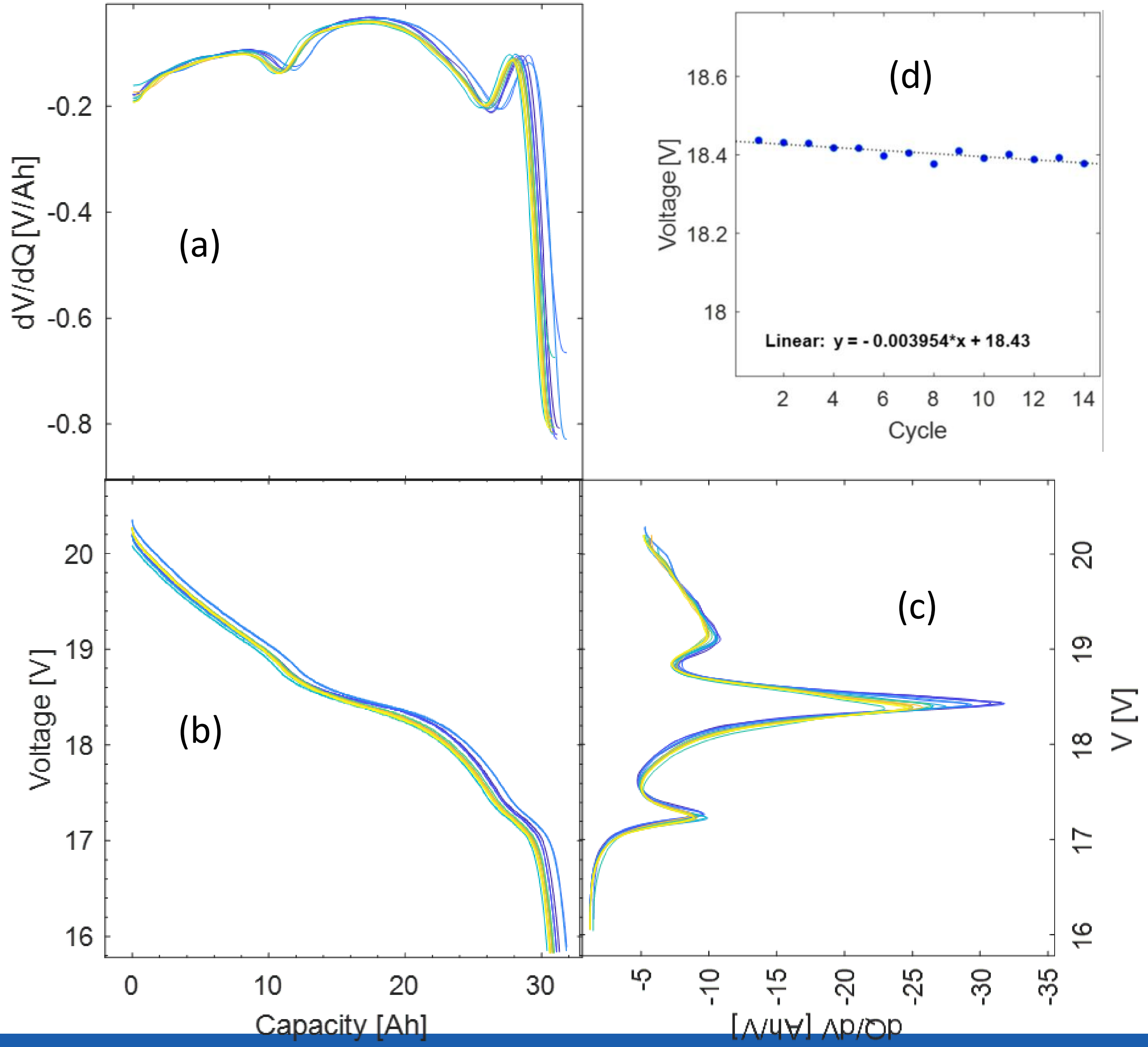
Pros:

1. Trends to well-known heuristics can be followed (e.g., $t^{1/2}$ law for capacity fade during calendar aging).
2. Anomalies can be detected (cycles 7 and 8; there was loss of data between the end of charge and beginning of discharge).
3. They are directly measurable from the on-orbit autocycle protocol.

Cons:

1. Lumped parameters: limited interpretability (R_{eff}); limited granularity (both).
2. Limited diagnostic power: cannot deconvolve or distinguish between key physical degradation modes like LLI vs. LAM.
3. Limited ability to detect early-stage faults due to "masking effect“.

Conventional Analysis: DVA. LLB-2#1005



Pros (in the lab):

1. A direct window into electrode thermodynamics.
2. Directly measures physical degradation modes like LLI and LAM

Cons (on-orbit):

1. Requires slow, "quasi-equilibrium" data (e.g., C/25) that is not available from on-orbit operations.
2. C/9 operational data distort and obscure the thermodynamic features (d).
3. Highly sensitive to measurement noise, making it "unreliable" for operational data.

Conventional Analysis: summary of limitations

1. **R & Q Metrics:** Lack the diagnostic power to distinguish between the underlying physical causes of degradation.

2. **DVA:** Is too sensitive to operational conditions (high-rates and noise), making it unreliable on the available on-orbit data.

A robust method is required to reliably extract
- **the maximum number of interpretable features**
- **from the available data**

Systematic model reduction. LLB-2 pack

Approximation: autocycle discharge=OCV;
Assumptions: cells are identical in the pack;

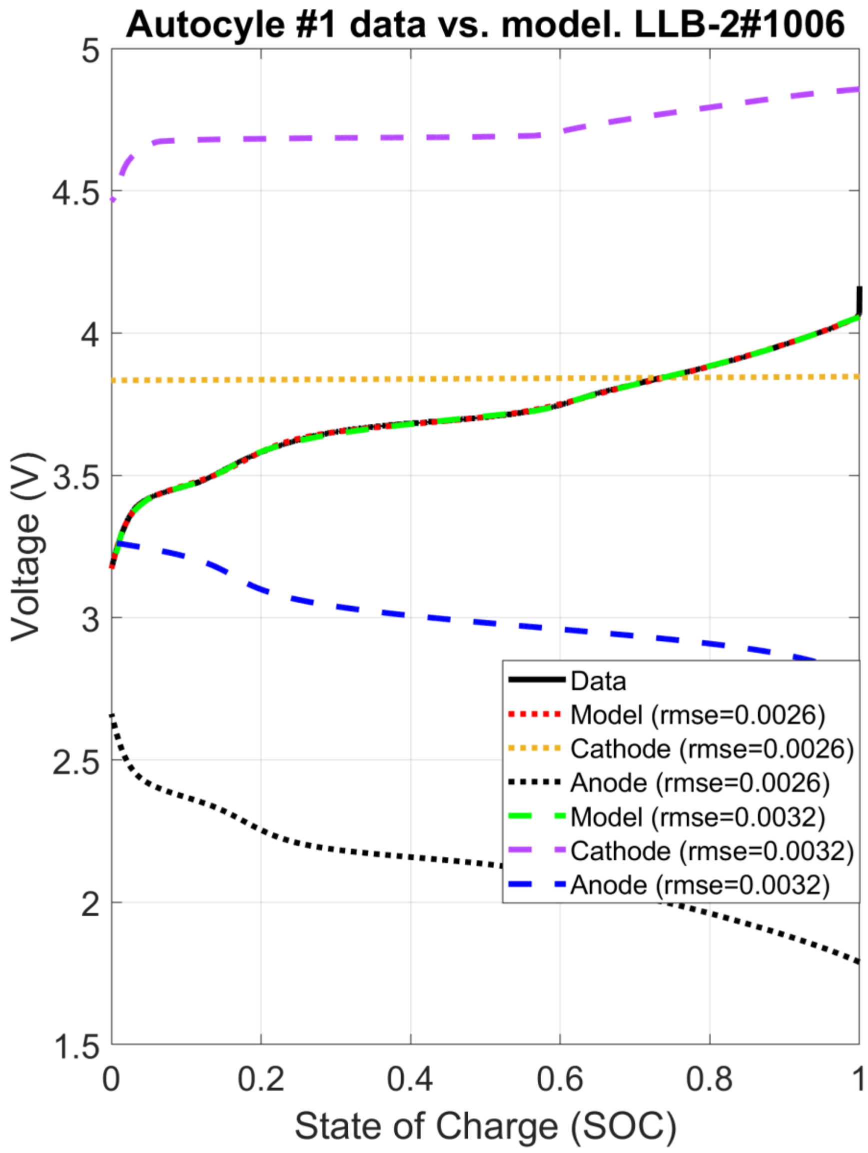
Initial full-order (**FOM**) physics-based model of electrode OCV, Verbrugge(2003), Birkl(2015):

$$x(E^{OC}) = \sum_{i=1}^{N} \frac{\Delta x_i}{1 + \exp\left((E^{OC} - E_{0,i})a_i e/kT\right)}$$

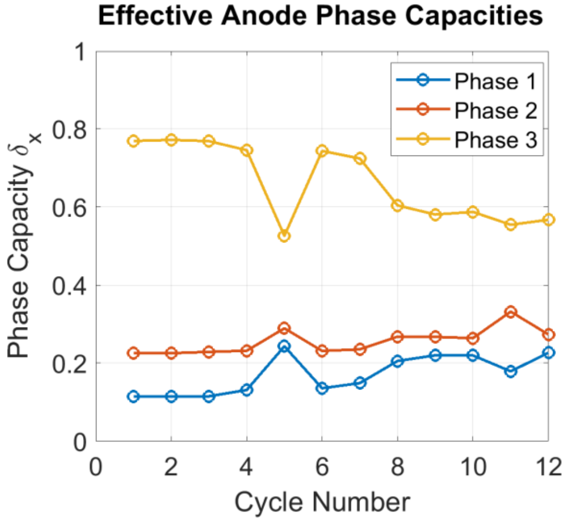
For two electrodes ~**30 parameters total**.

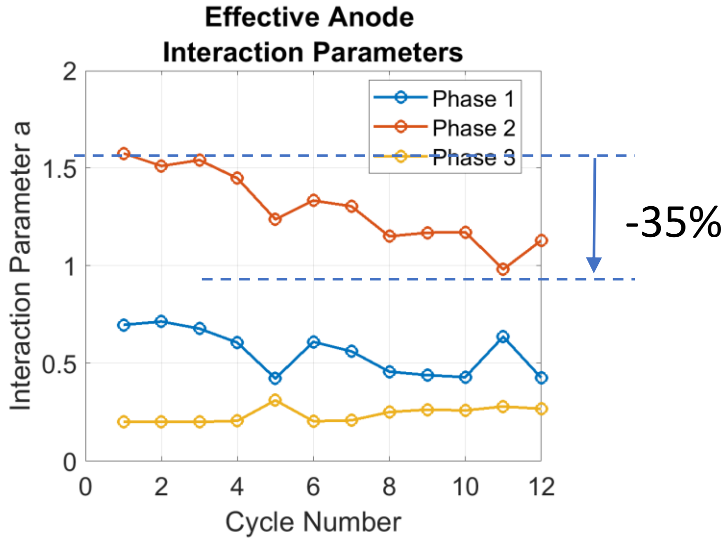
The model is **non-identifiable** from the OCV data (see the Figure).

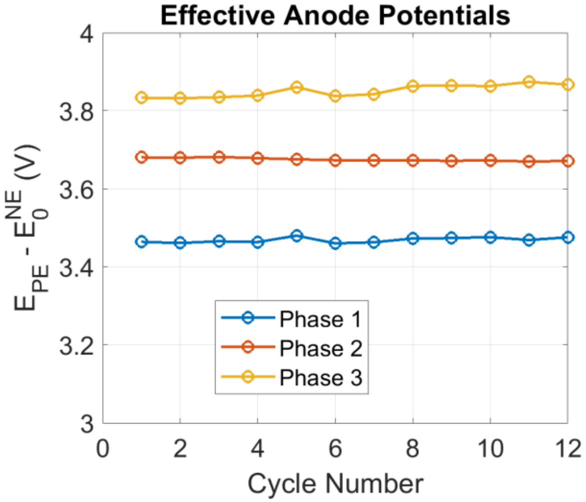
Reduction leads to an identifiable **9-parameter OCV model**

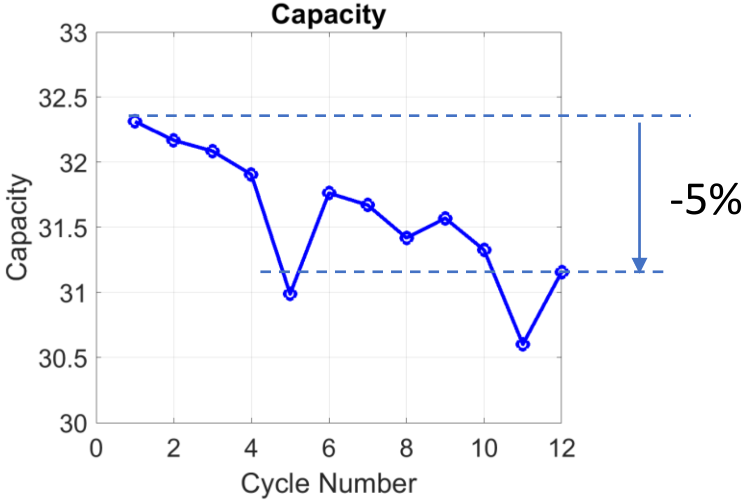


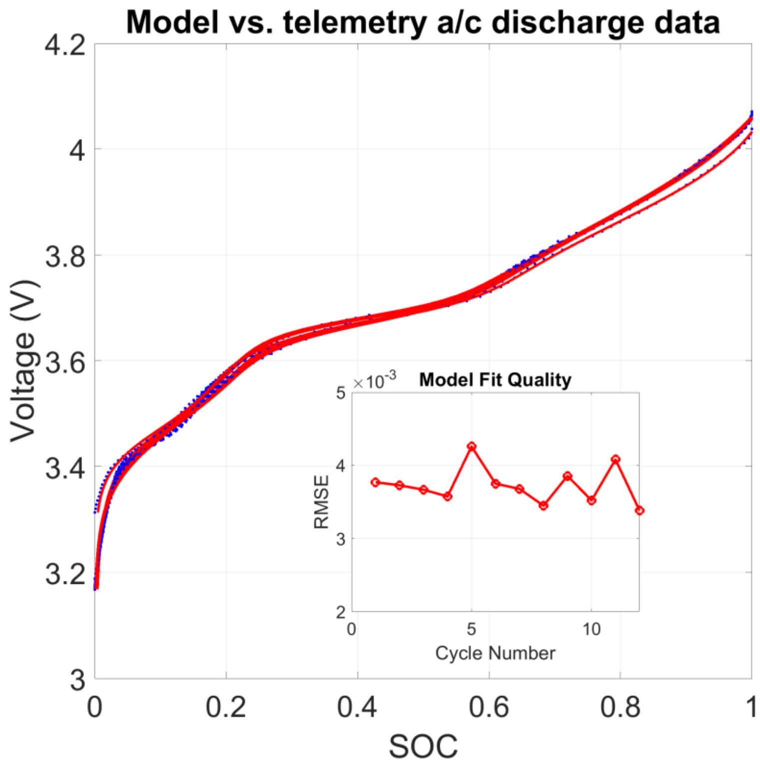
9pROM-I parameter evolution. ISS; **LLB-2#1006**





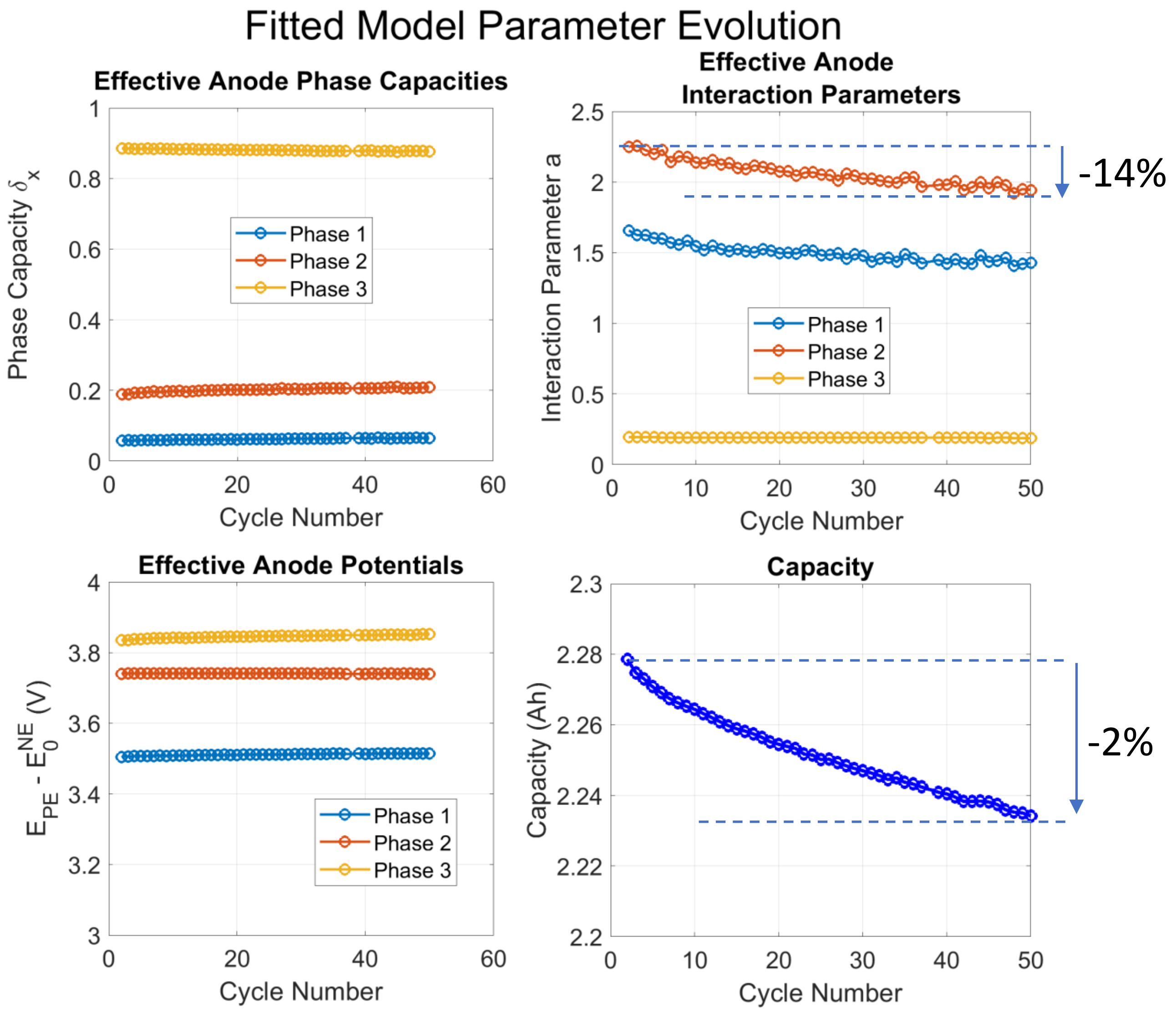


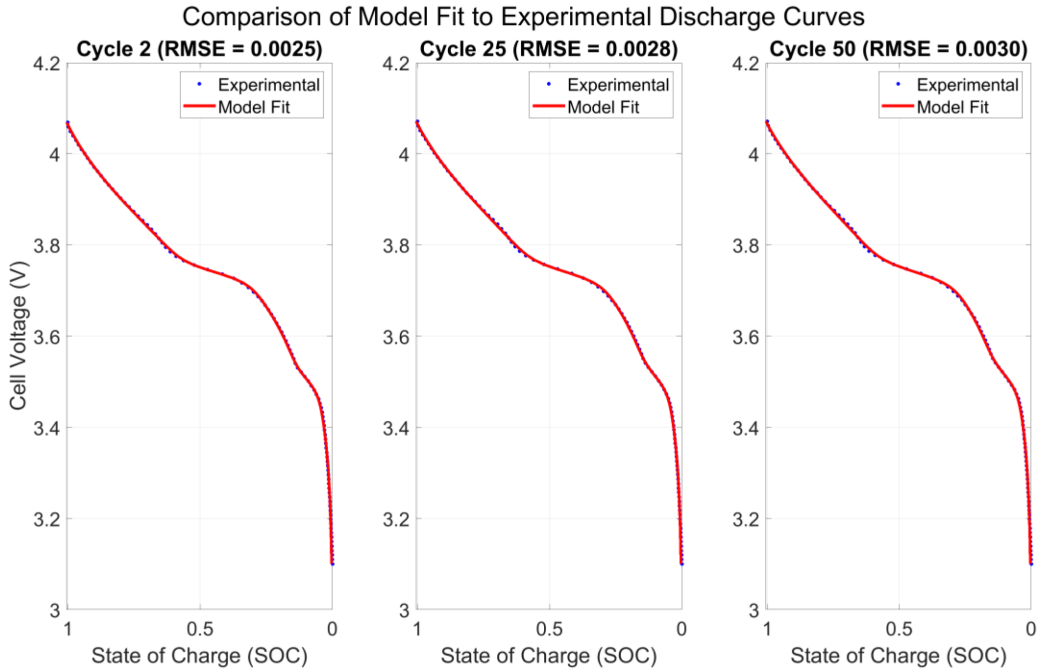




- ✓ 9pROM-I is accurate (RMSE< 0.5%) and identifiable from telemetry data
- ✓ 9 parameters are being monitored (on top of capacity and resistance)
- ✓ Evolution shows anomalies at cycle 5 and 11 (resolved)
- ✓ Phase-I effective anode interaction parameter is highly sensitive to aging

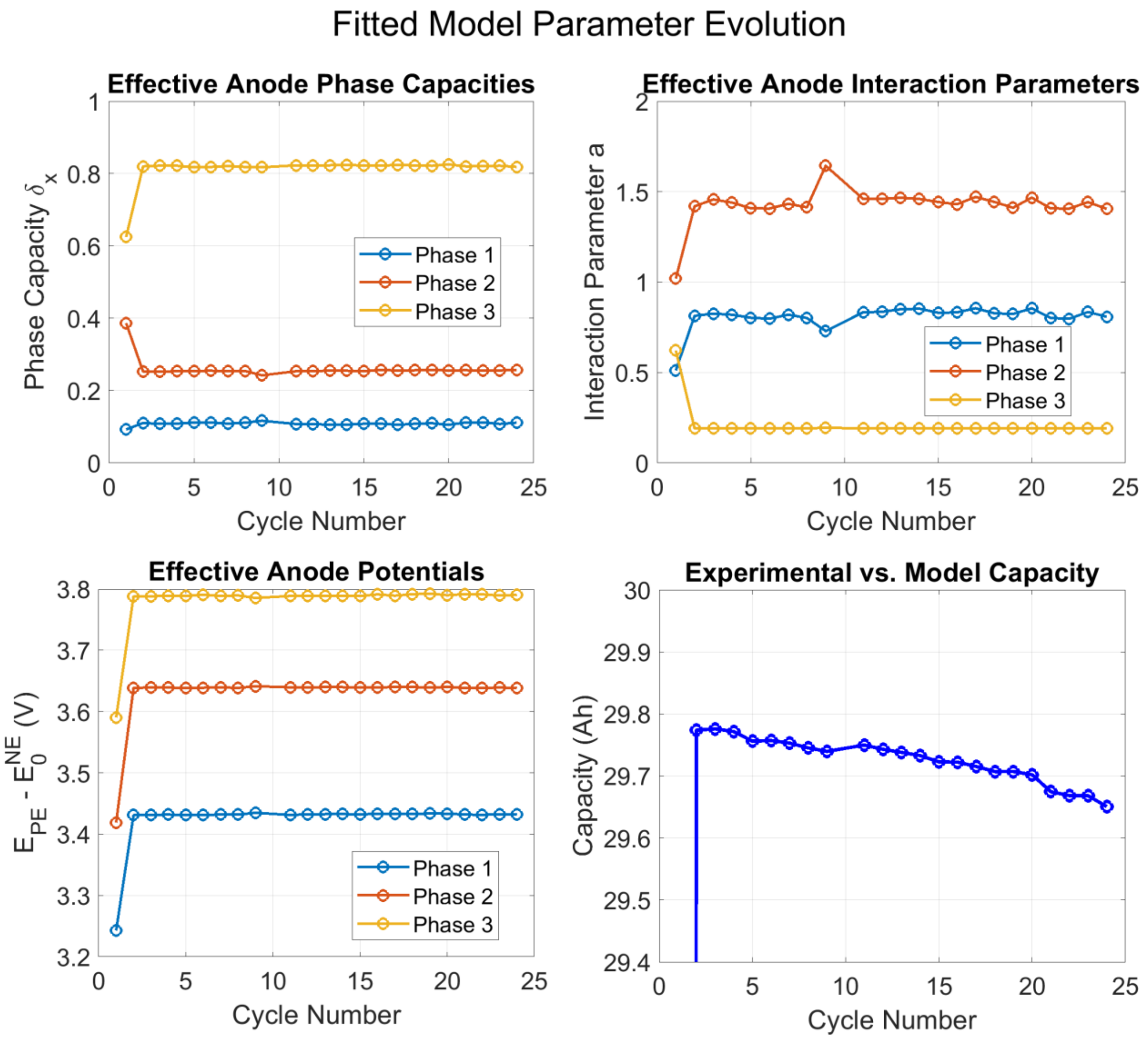
9pROM-I parameter evolution. Ambient cycling; **SRI cells**

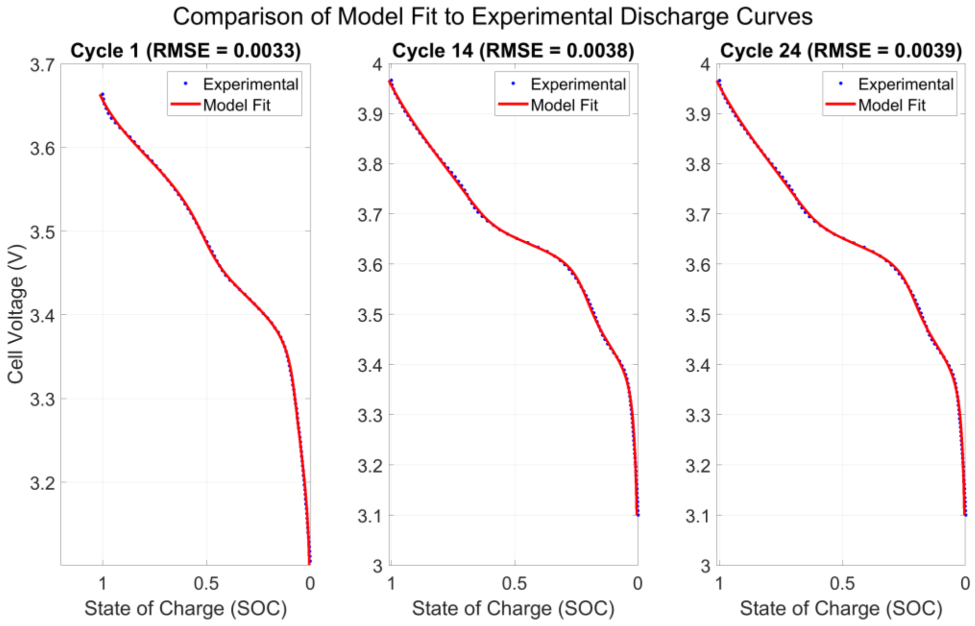




- ✓ 9pROM-I is accurate and identifiable
- ✓ 9 parameters are being monitored (on top of capacity and resistance)
- ✓ Evolution does not shown anomalies
- ✓ Phase-I effective anode interaction parameter is highly sensitive to aging

9pROM-I parameter evolution. Ambient; **LLB-2#1001**





- ✓ 9pROM-I is accurate and identifiable
- ✓ 9 parameters are being monitored (on top of capacity and resistance)
- ✓ Outliers: cycle 1 and 9

Summary

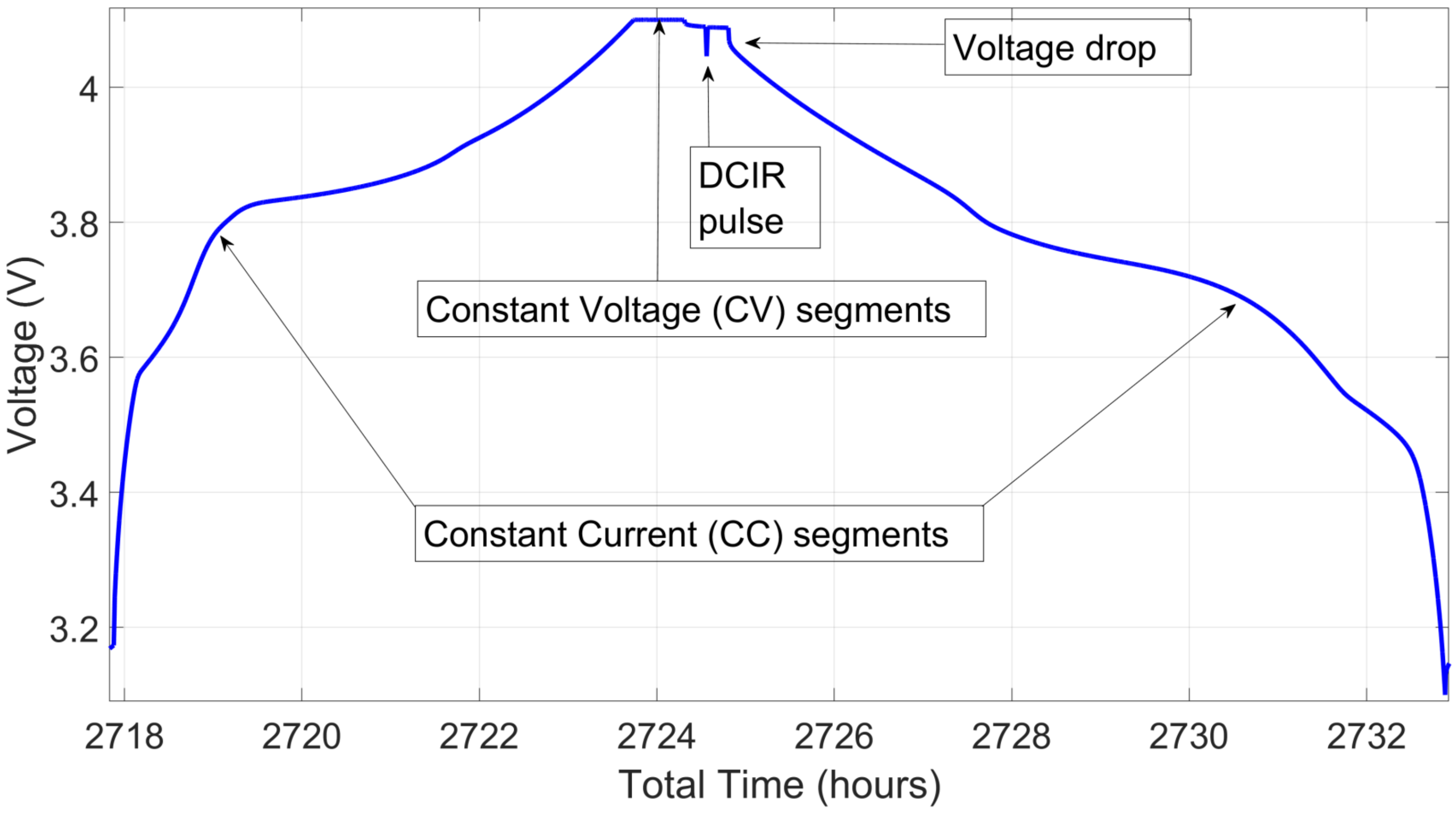
RESULTS

- **Physics-based ROM** for LLB-2 cell telemetry complete:
  - ✓ Accurate (≤ 0.5 % RMSE)
  - ✓ Identifiable (9 par + Q + R)
- Observed anomalies resolved (gaps in data)

REMARKS

- **Assumption:** OCV
  - ✓ Conflates thermodynamics features with kinetic effects
  - ✓ Ignores kinetic features of the data (voltage smoothing, voltage drop)
  - ✓ Ignores kinetic data (voltage relaxation post EVA)
- **Essentially equivalent** to DVA but robust and explicitly T-dependent (relevant for ESTA data)
- **Masking effect:** cell to cell variations cannot be resolved
- **Limited Remaining Useful Life prediction** can be made due to the limited storage aging data for LLB-2.

Data segments



- Each segment is modeled separately
- CV, DCIR and voltage drop models have been validated
- CC segment model is being currently validated

Constant current (CC) model

$$\theta_i(\phi_i) = \sum_{j=1}^{N_i} \frac{\delta_{i,j}}{1 + \exp\left[\frac{e a_{i,j}}{k_B T}(\phi_i - \varepsilon_{i,j})\right]},$$

OCV model, validated in earlier work

$$V(t) = \phi_c(\theta_c^{(0)}(t)) - \phi_a(\theta_a^{(0)}(t))$$

$$+ \left.\frac{\partial \phi_c}{\partial \theta_c}\right|_{\theta_c^{(0)}(t)} \frac{I(t)\,\tau_c}{15\,eM_c} + \left.\frac{\partial \phi_a}{\partial \theta_a}\right|_{\theta_a^{(0)}(t)} \frac{I(t)\,\tau_a}{15\,eM_a}$$

$$- \frac{2k_BT}{e} I(t) \left(\frac{1}{\tilde{I}_{e,c}\sqrt{\theta_c^{(0)}(t)(1-\theta_c^{(0)}(t))}} + \frac{1}{\tilde{I}_{e,a}\sqrt{\theta_a^{(0)}(t)(1-\theta_a^{(0)}(t))}} \right) - R_\Omega I(t).$$

$$\theta_a^{(0)}(t) = \theta_{a,0} - \frac{1}{eM_a}\int_0^t I(t')\,\mathrm{d}t', \qquad \theta_c^{(0)}(t) = \theta_{c,0} + \frac{1}{eM_c}\int_0^t I(t')\,\mathrm{d}t'$$

SPM for low current

$\{\delta_{i,j}, a_{i,j}, \varepsilon_{i,j}\}_{i=a,c;\, j=1,\ldots,N_i}$, τ_a, τ_c, $\tilde{I}_{e,a}, \tilde{I}_{e,c}$, R_Ω, M_a, M_c, $\theta_{a,0}, \theta_{c,0}$, ~ 20 parameters

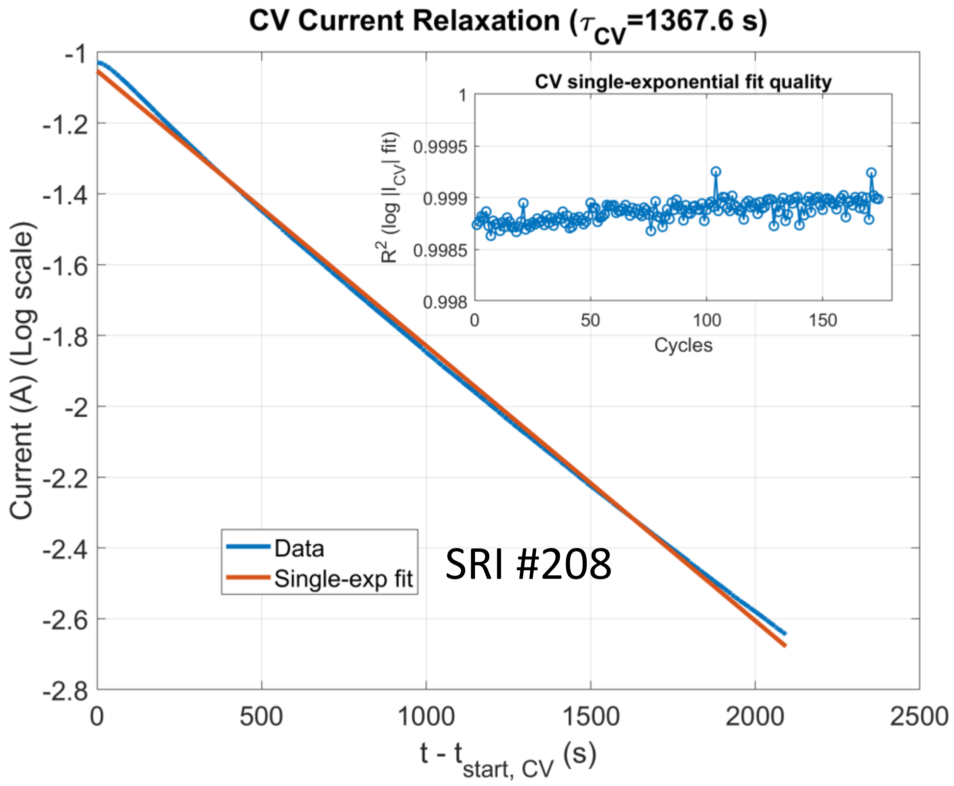
Constant voltage (CV) model

Based on the SPM and known properties of graphite anodes OCV at high SOC derived the following CV model

Ohmic + charge-transfer kinetic resistance

$$I(t) \approx I_0 \exp(-t/\tau_{\mathrm{CV}}), \qquad \tau_{\mathrm{CV}} = \frac{R_{\Omega+ct}\, eM_c}{-\dfrac{\mathrm{d}\phi_c}{\mathrm{d}\theta_c}},$$

Cathode pseudo-capacitance



- The model was validated on ambient SRI and Freezer cell data.
- The model allows to infer **τ**, interpretable in terms of fundamental (SPM) physical parameters.
- Given $\mathbf{R_{\Omega+ct}}$ (inferred from the DCIR + Voltage drop models) cathode pseudocapacitance can be inferred.
- Finite **τ** imposes constrain on the cell's OCV parameters as cathode OCV must have finite slope
- Current **I(t)** allows to compute initial $\boldsymbol{\theta_a}$ and $\boldsymbol{\theta_c}$ for the discharge branch of the CC model

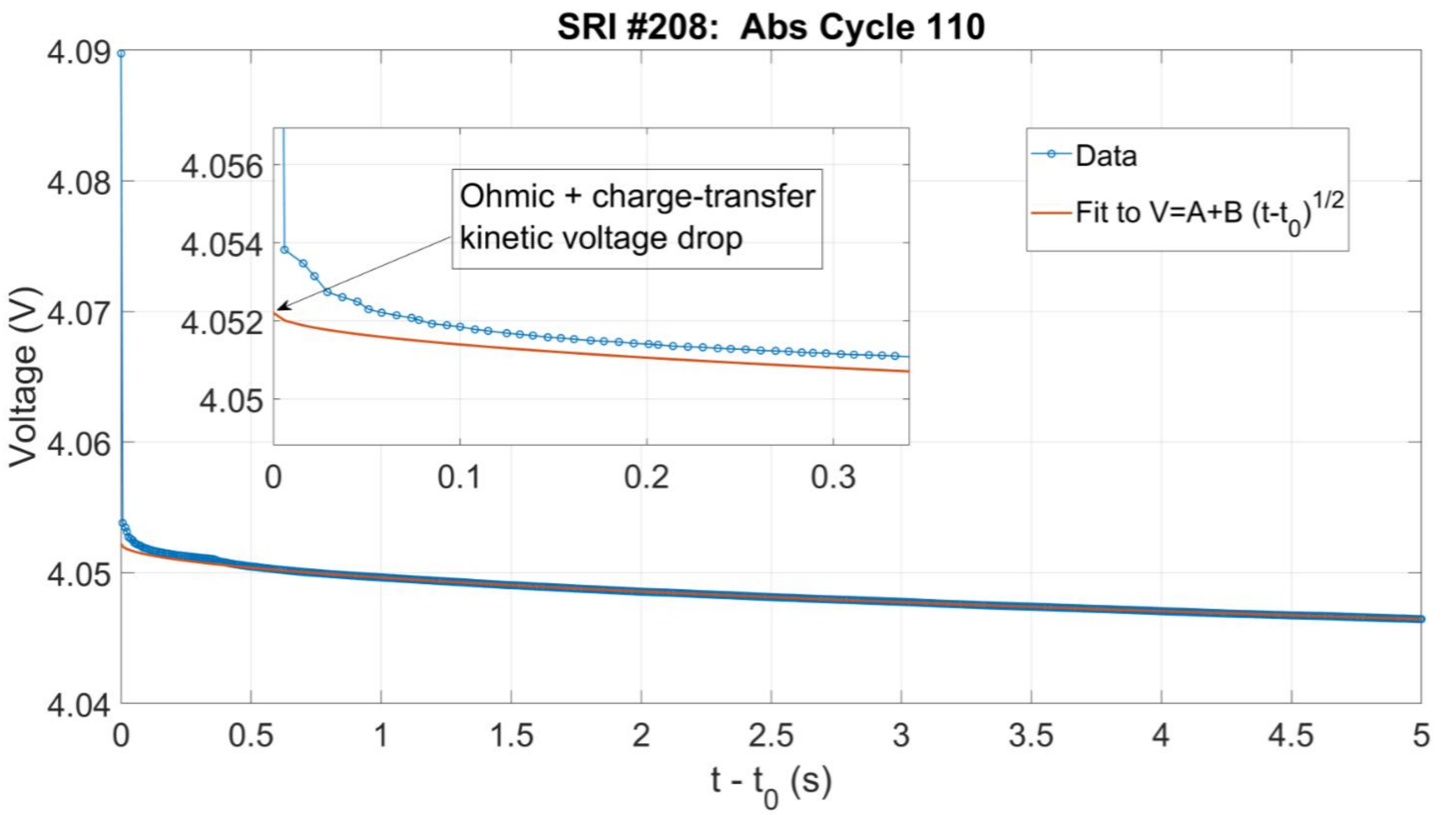
DCIR model

Voltage drop under DC pulse gives:

$$R_{exit} \equiv \frac{\Delta V_{exit}}{I_{pulse}} = R_{\Omega+ct} + R_{diffusion}$$

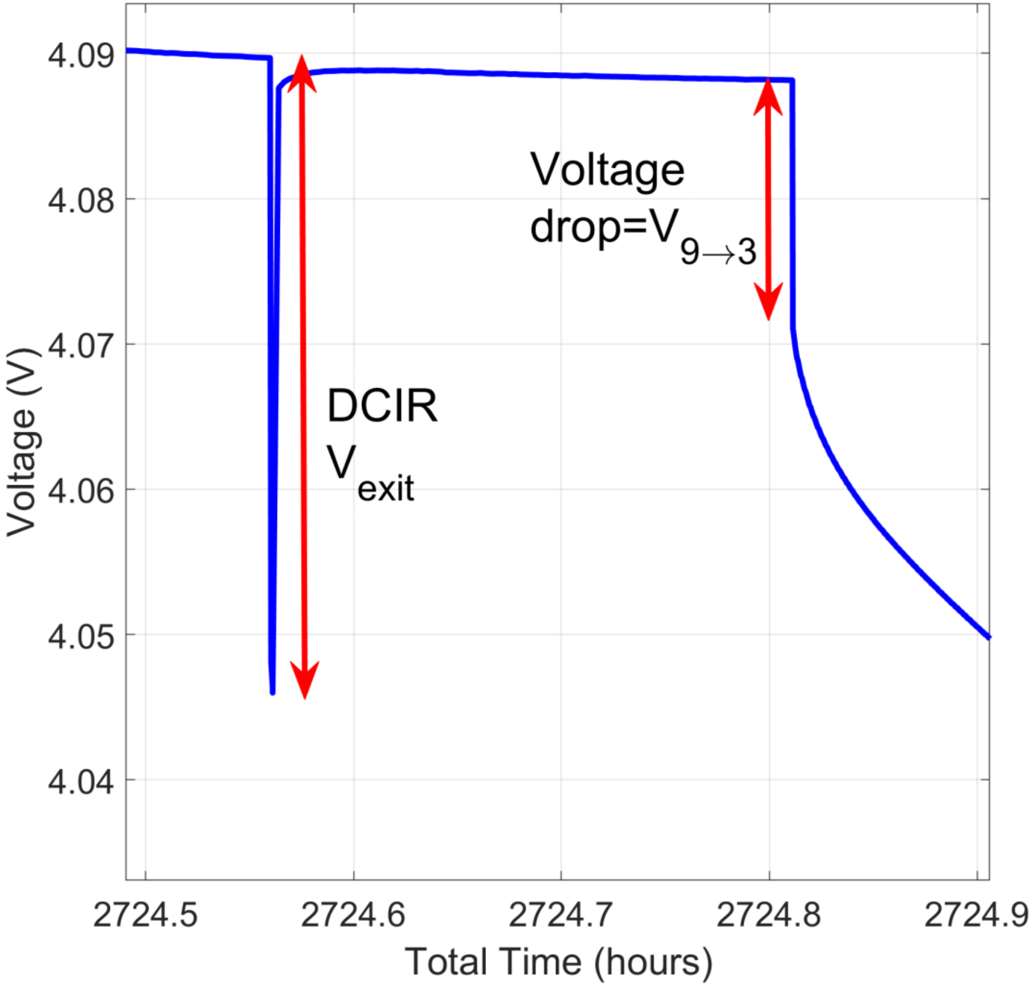
$R_{diffusion}$ can be derived from the SPM:

$$R_{diffusion} = \frac{2}{3e}\sqrt{\frac{\Delta t}{\pi}}\left[\frac{\sqrt{\tau_c}}{M_c}\left|\frac{\partial \phi_c}{\partial \theta_c}\right| + \frac{\sqrt{\tau_a}}{M_a}\left|\frac{\partial \phi_a}{\partial \theta_a}\right|\right], \quad \Delta t \ll \tau_c, \tau_a.$$



- The model was validated on ambient SRI and Freezer cell data.
- Extrapolating **$R_{diffusion}$(t)** to the beginning of the pulse we can infer **$R_{\Omega+ct}$**.
- Therefore, the model allows to infer two lumped parameters, which are known functions of the fundamental (SPM) parameters.
- At ISS ΔV(t) is not measured; therefore extrapolation is not possible.
- However, both **$R_{diffusion}$** and **$R_{\Omega+ct}$** can be inferred jointly from DCIR + discharge voltage drop model.

Discharge voltage drop model and joint (with DCIR model) inference



Inputs:

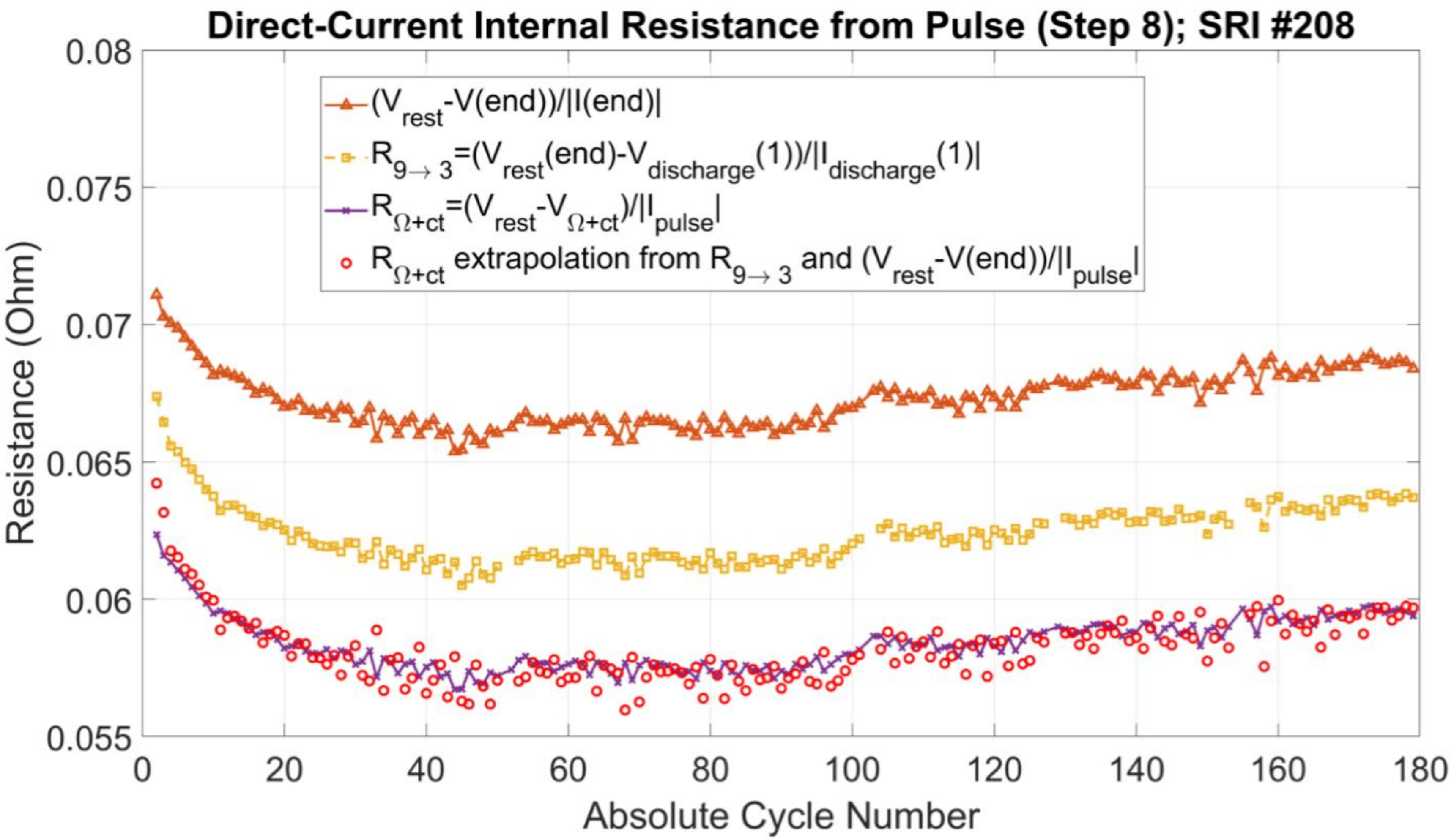
1. Voltage drops in the beginning of discharge and end of DCIR pulse (available at ISS)
2. DCIR pulse current and discharge current
3. Duration of the DCIR pulse and the sampling rate at CC discharge

Outputs:

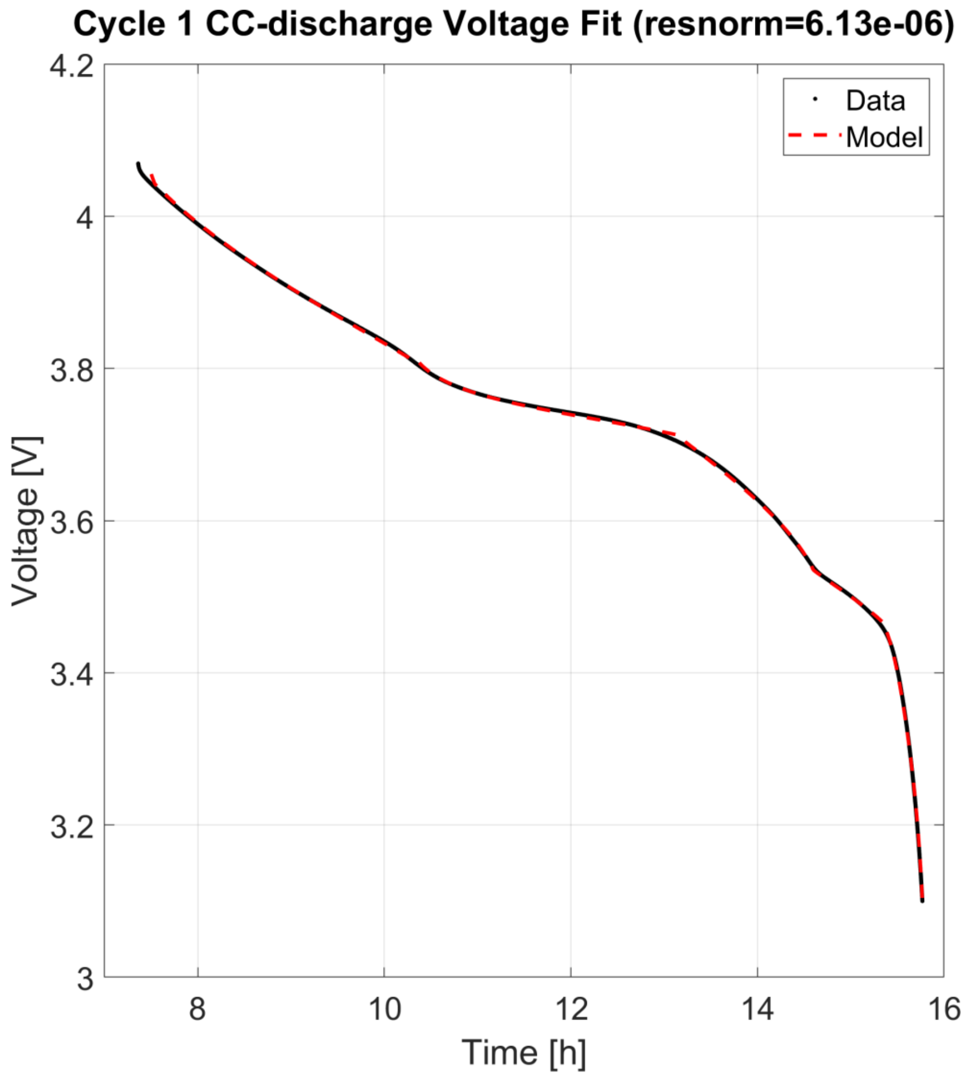
$$R_{\Omega+ct} \approx \frac{R_{9\to3}\sqrt{t_{\mathrm{exit}}} - R_{\mathrm{exit}}\sqrt{t_{9\to3}}}{\sqrt{t_{\mathrm{exit}}} - \sqrt{t_{9\to3}}},$$

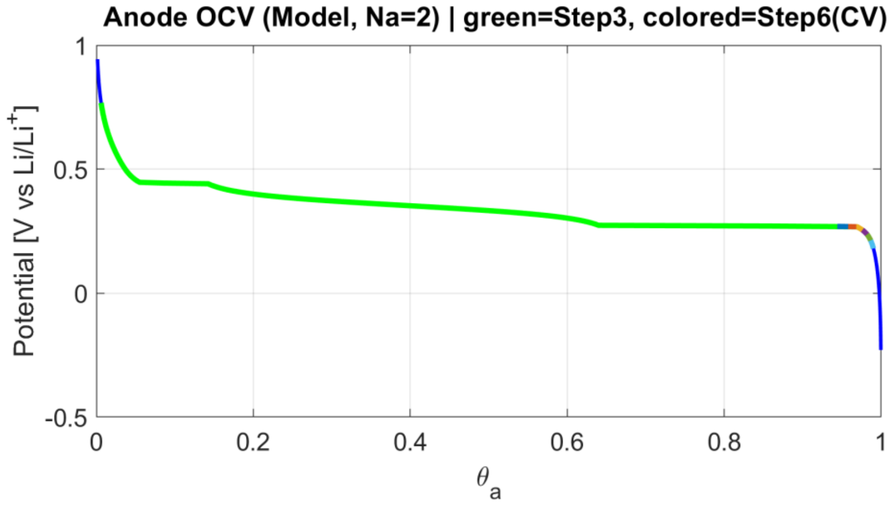
$$R_{\mathrm{diff}} \approx \frac{R_{\mathrm{exit}} - R_{9\to3}}{\sqrt{t_{\mathrm{exit}}} - \sqrt{t_{9\to3}}}\sqrt{t_{\mathrm{exit}}}.$$

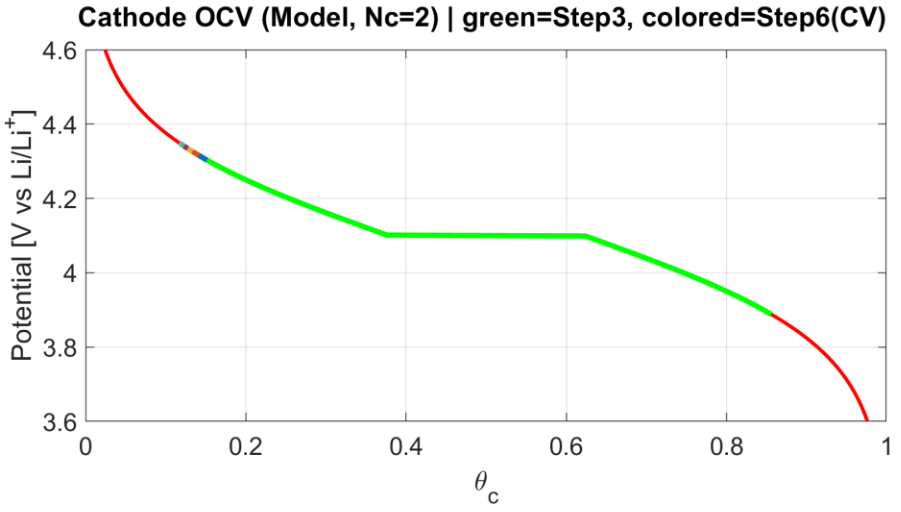
Voltage drop model and joint (with DCIR model) inference



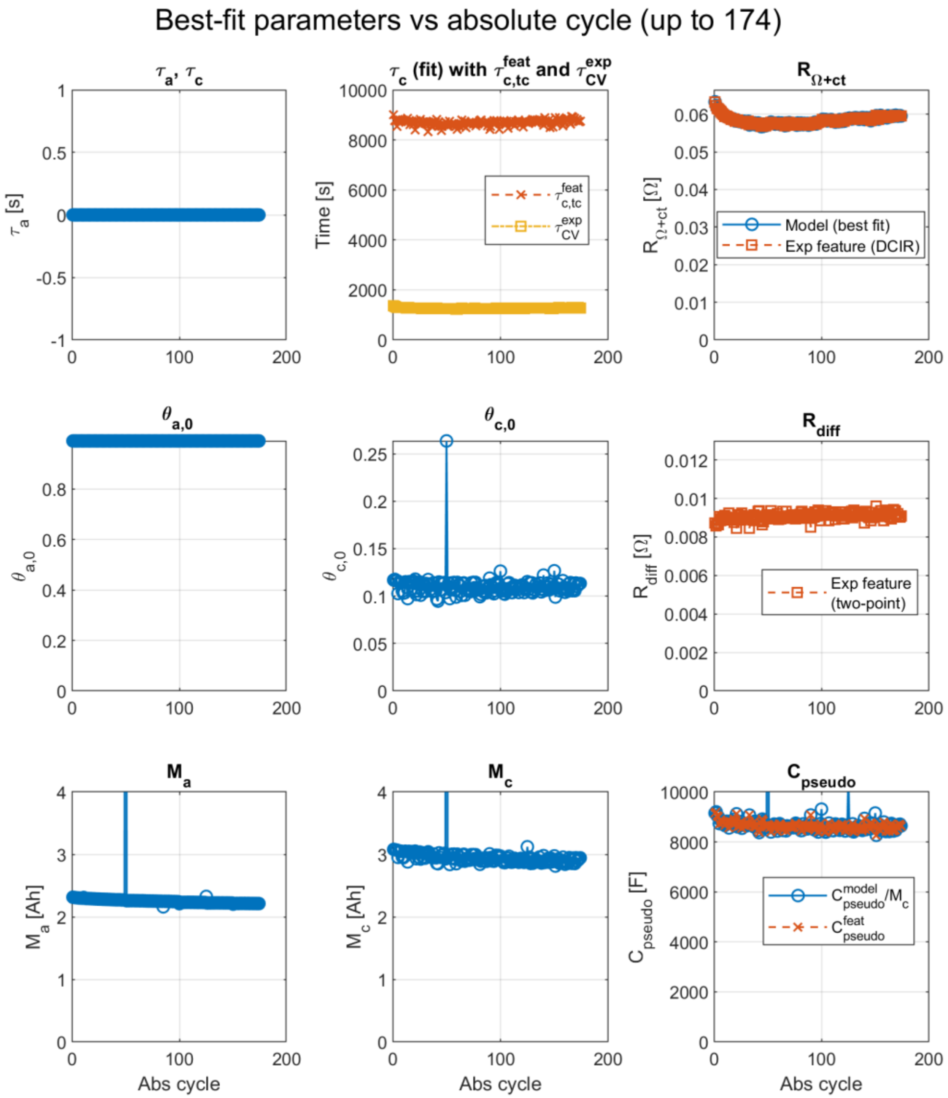
ROM accuracy

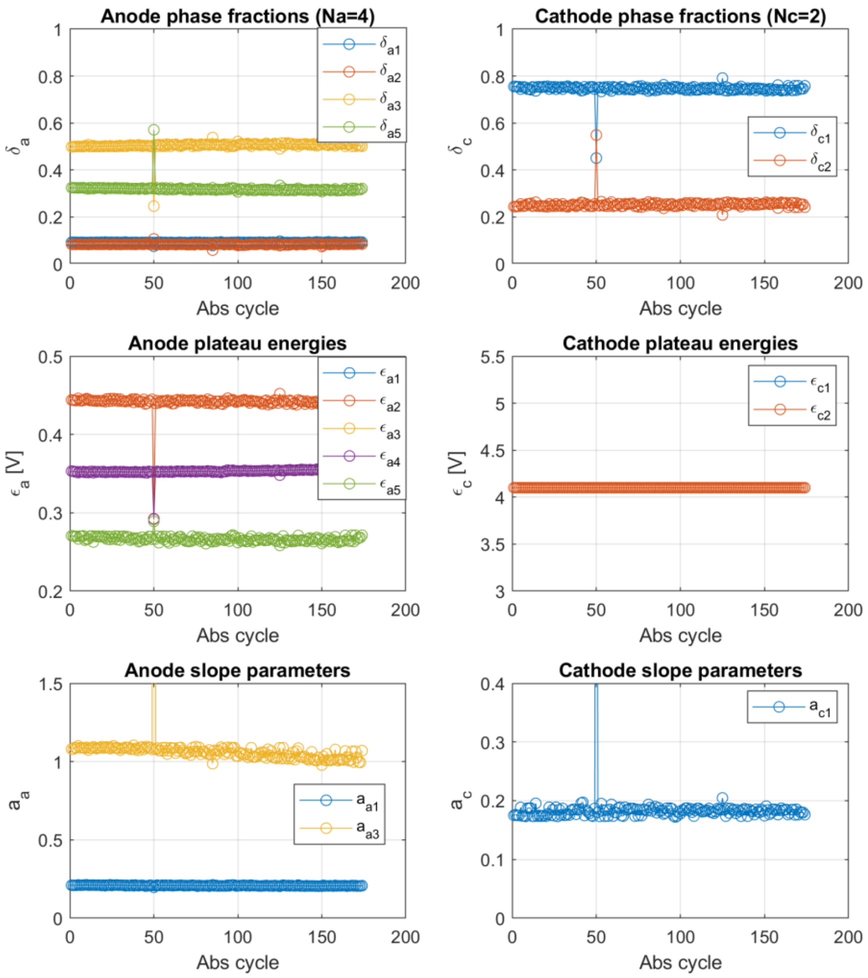






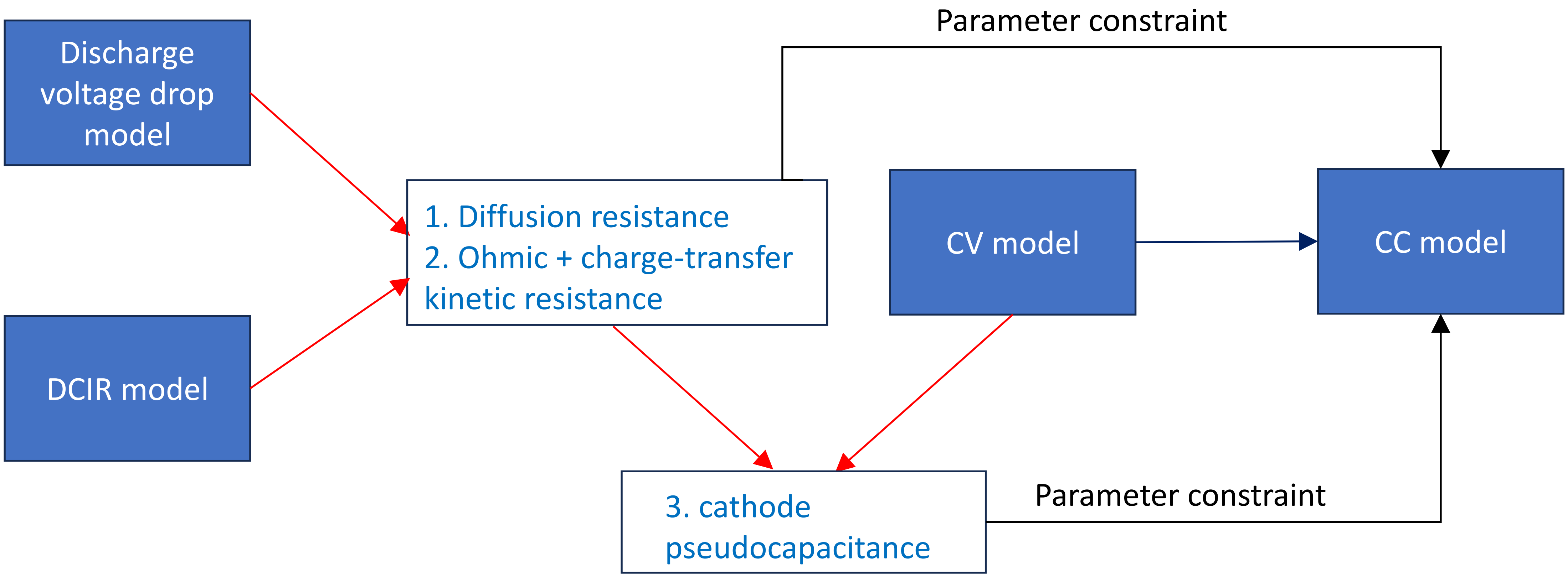
Parameter inference for SRI cells





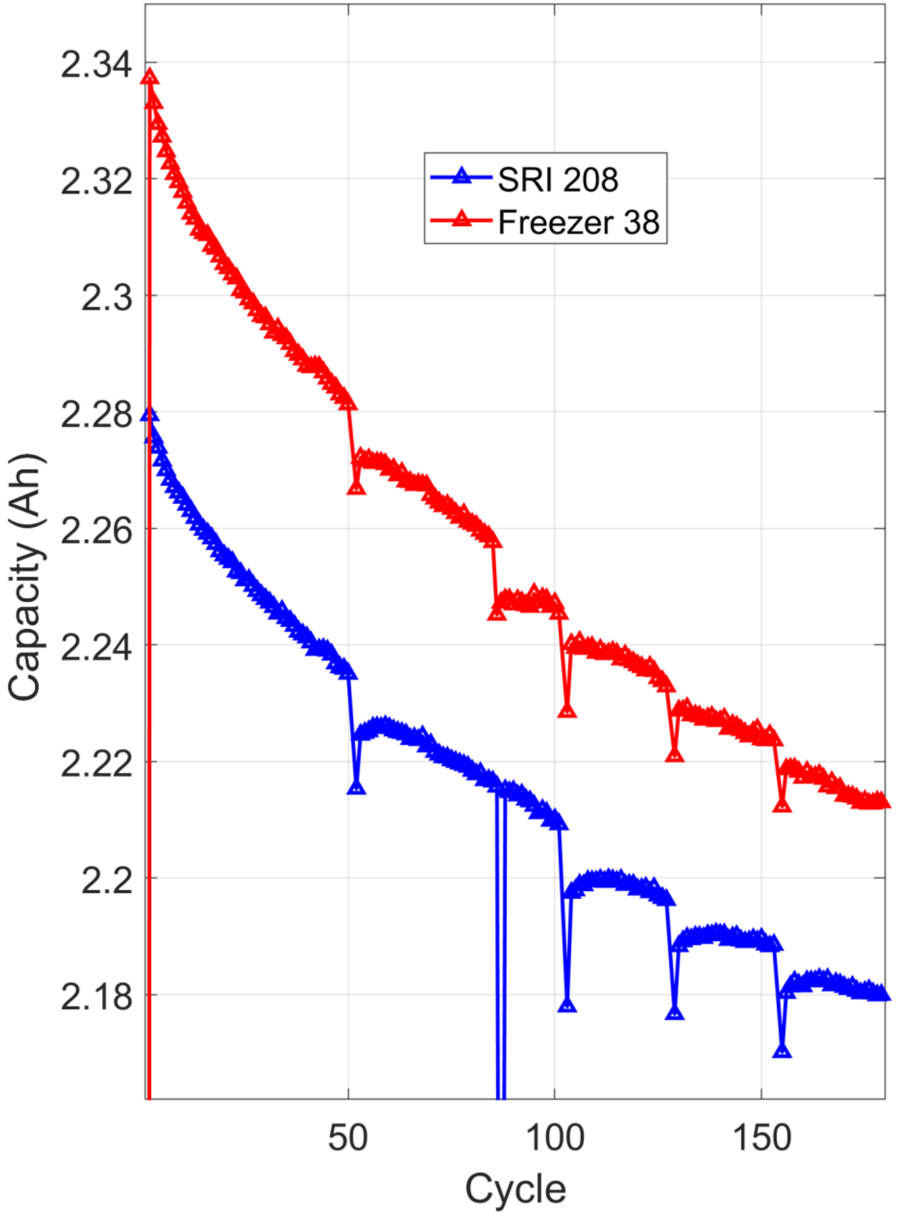
17 parameters can be inferred

Models' interconnection



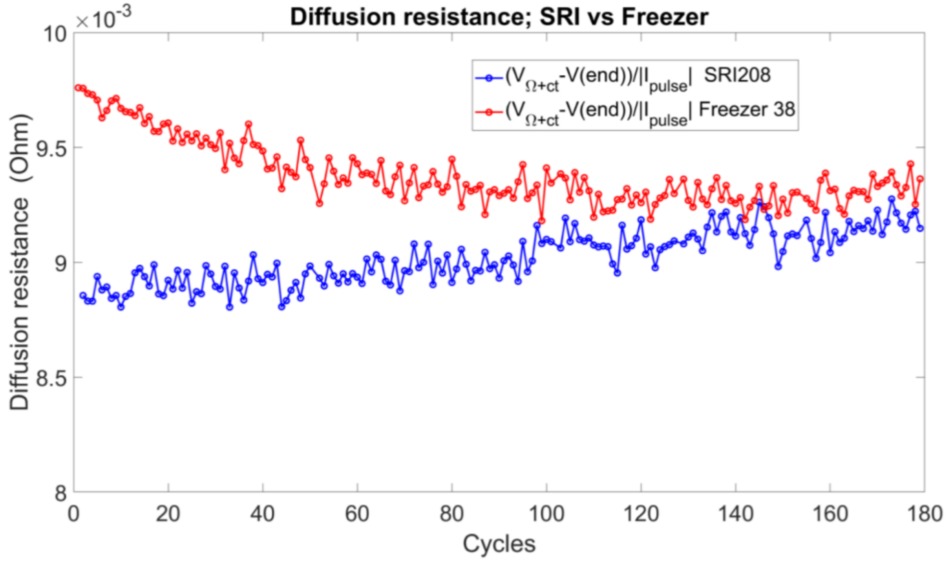
Preliminary data analysis: SRI vs Freezer cells

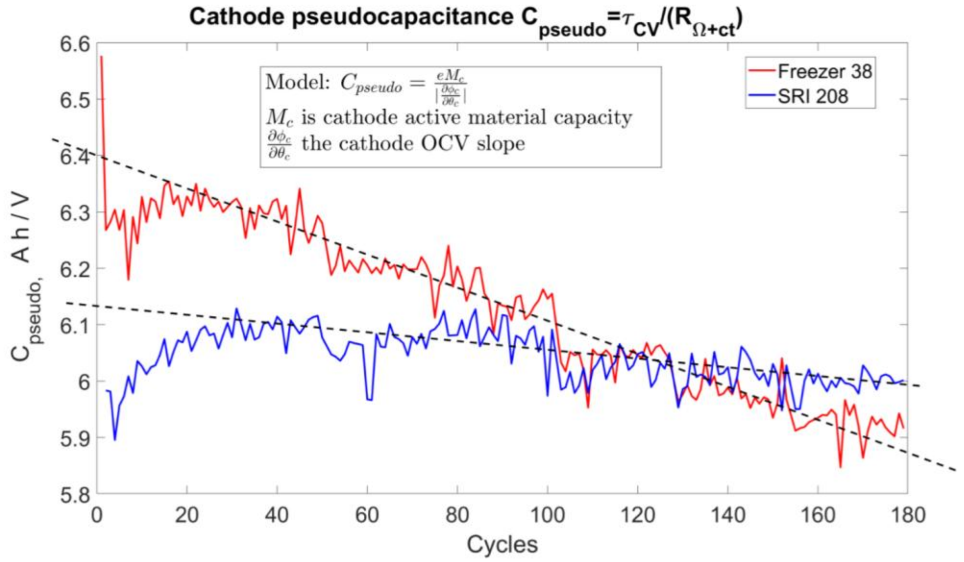
The overhang effect

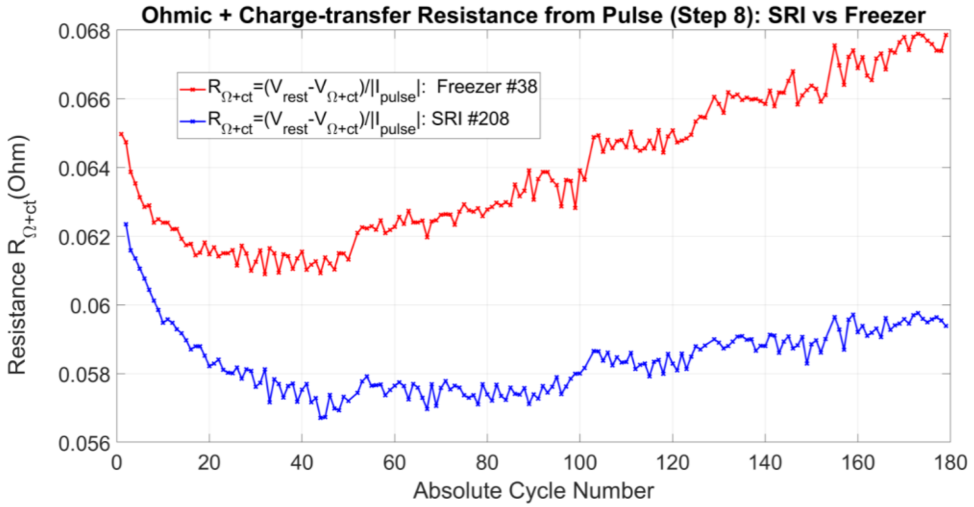


1. Freezer: amplitude of the overhang is smaller
2. Hypothesis: manufacturing differences between the Freezer (2016 lot) and SRI (2013 lot); e.g., overhand length of 1mm vs 0.3mm.
3. Can be confirmed using CT or DPA

Resistances and cathode pseudocapacitance at 4.1V







1. Freezer and SRI cells exhibit opposing trends in the diffusion resistance
2. Freezer cells have higher rate of the ohmic+charge-transfer kinetic resistance growth
3. Freezer cells have higher rate of the pseudocapacitance decay
4. All the trends can be explained by the fact that Freezer cells start cycling campaign at higher capacity (lithium inventory) due to the difference in the storage conditions