Development of Reduced-Order Models for Li-ion Battery Performance Predictions

Albert H. Zimmerman and
Christopher S. Choi
The Aerospace Corporation

20 April 2021
Space Power Workshop

Note: Pictures, Graphs and Diagrams shown
on the briefing charts are notional items, not exact.

Outline of Presentation

- Discussion of methods for predicting battery performance
- The approach planned for this project
- Description of the Reduced-Order-Model (ROM)
- Data-based assembly of a ROM
- Modeling Results
- Future Plans
- Conclusions

Battery Performance Prediction Methods

- **Look-up tables based on test performance**
  - *Test matrix must include all profiles of interest*
  - *Testing must be repeated periodically as cells age*
- **Life-test trends for voltage, resistance, and capacity**
  - *Not easily extended to profiles or conditions absent from life test*
- **Semi-empirical models**
  - *Require numerous parameters*
  - *Must include all internal cell reactions and ageing processes*
- **First-principles models**
  - *Require numerous parameters*
  - *Complex coupled physical, electrochemical, and ageing processes*
  - *Significant computational overhead*

Our approach falls into the test-based semi-empirical portion of the spectrum

Computational complexity

Approach for This Project

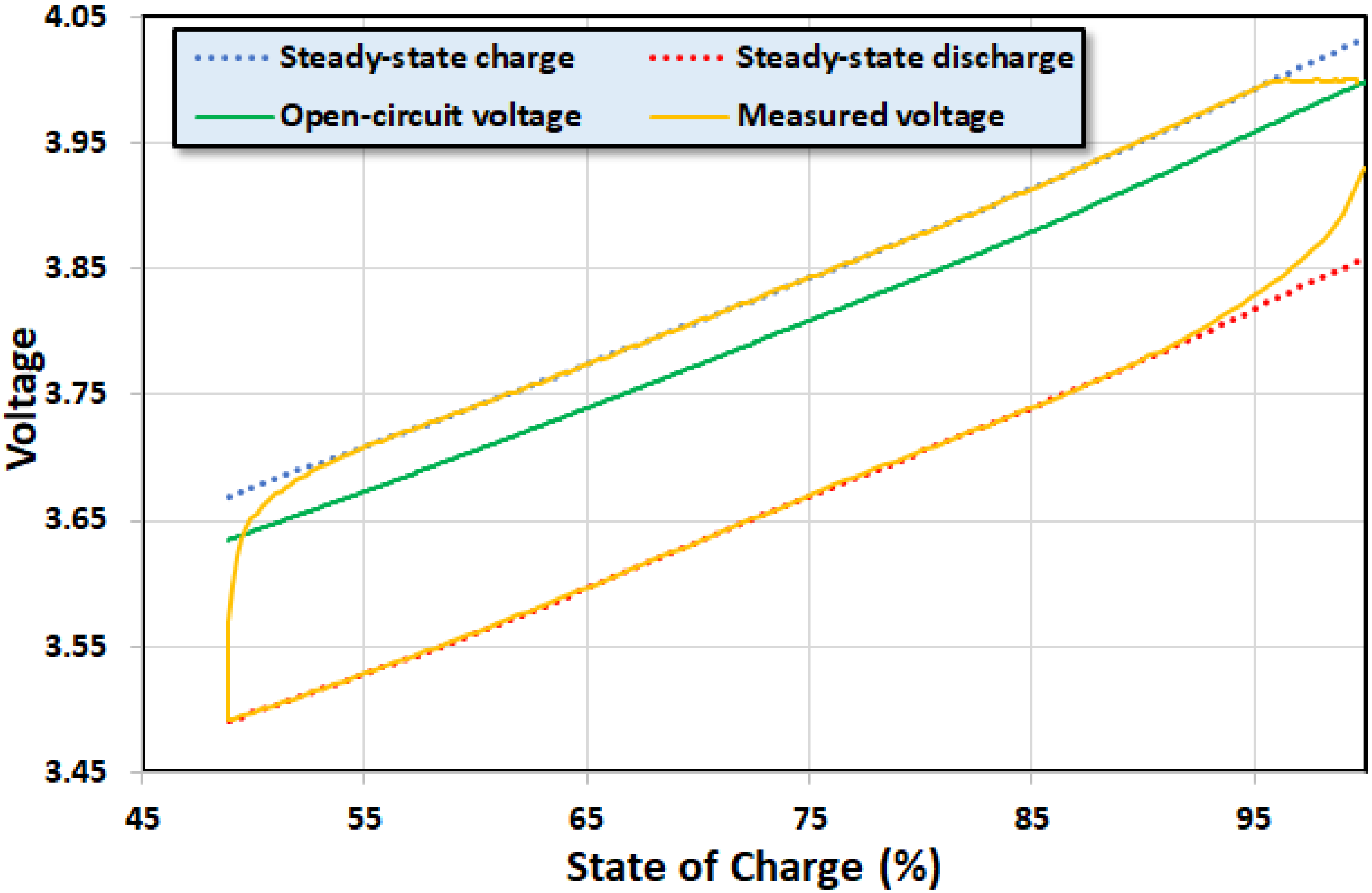
- **Develop a Reduced-Order-Model to describe Li-ion cell performance**
  - *Model allows cell data to describe all processes affecting performance and ageing*
  - *Take full advantage of large Li-ion life-test databases, i.e. allow the data to capture all necessary physics*
- **A ROM fully describes cell performance at any point in time**
- **A new ROM is generated for each point in time (each cycle)**
  - *Allows changes as cells age to be captured*
- **A new ROM is generated for each cell of interest**
  - *Can provide performance statistics from tests involving multiple cells*
- **A Long Short-Term Memory (LSTM) neural net is trained from life test databases**
  - *"Learns" the correct ROM to be applied for any condition*
  - *Capable of remembering performance during capacity checks or eclipse seasons that may occur only once or twice per year*
- **Trained LSTM net subsequently used to predict cell performance**

Description of the Reduced-Order-Model

- **What is the minimum physics that we need to guide the neural net?**
- **Key model elements obtained from each cycle (minimalist model)**
  - *Open circuit voltage as a function of cell state of charge (SOC)*
    - Describes electrochemical potentials and thermodynamics for reactions
  - *DC resistance as a function of SOC*
    - Describes kinetics of cell processes
  - *Lithium ion gradients in electrode materials*
    - Describes voltage transients during non-steady-state operation
  - *Cell capacity available*
    - From capacity measurements or open-circuit voltage trends
- **All degradation processes are described by changes in these elements as the cells age**
- **This model enables cell performance to be predicted for any charge/discharge current or power profile**

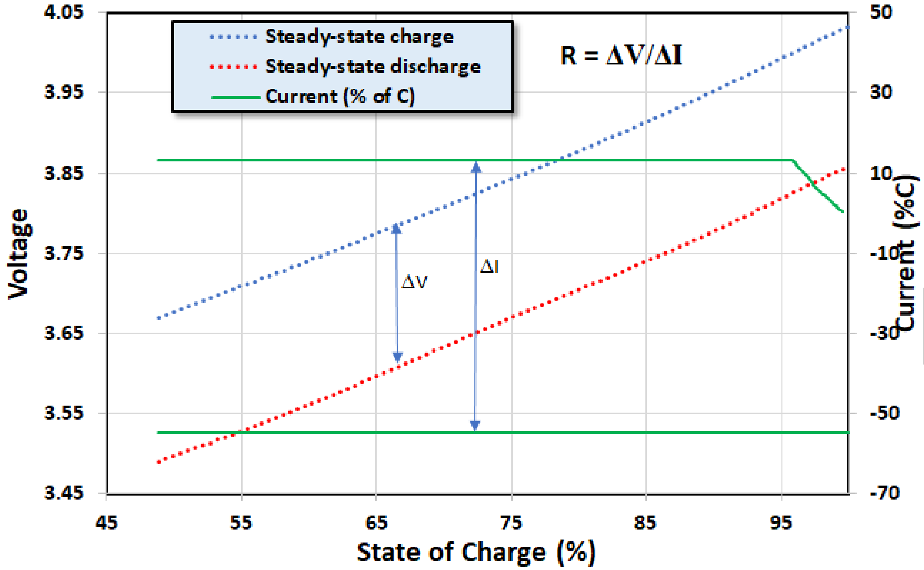
Evaluation of the Open Circuit Voltage

- **Based on Ohm's Law interpolation* between steady-state charge and discharge voltages (example shown for 52% DOD cycle)**



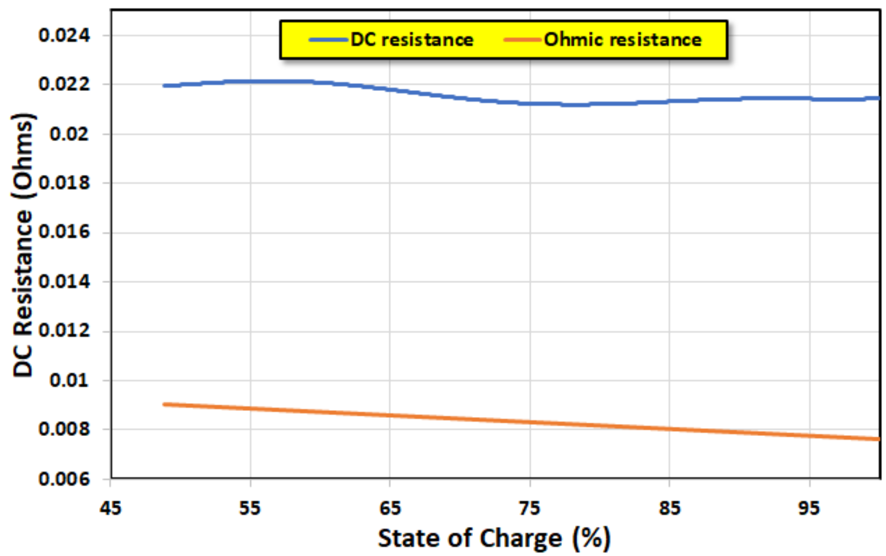
**Assumes cell operation at low charge transfer overpotentials (typical for Li-ion)*

Evaluation of the DC Resistance



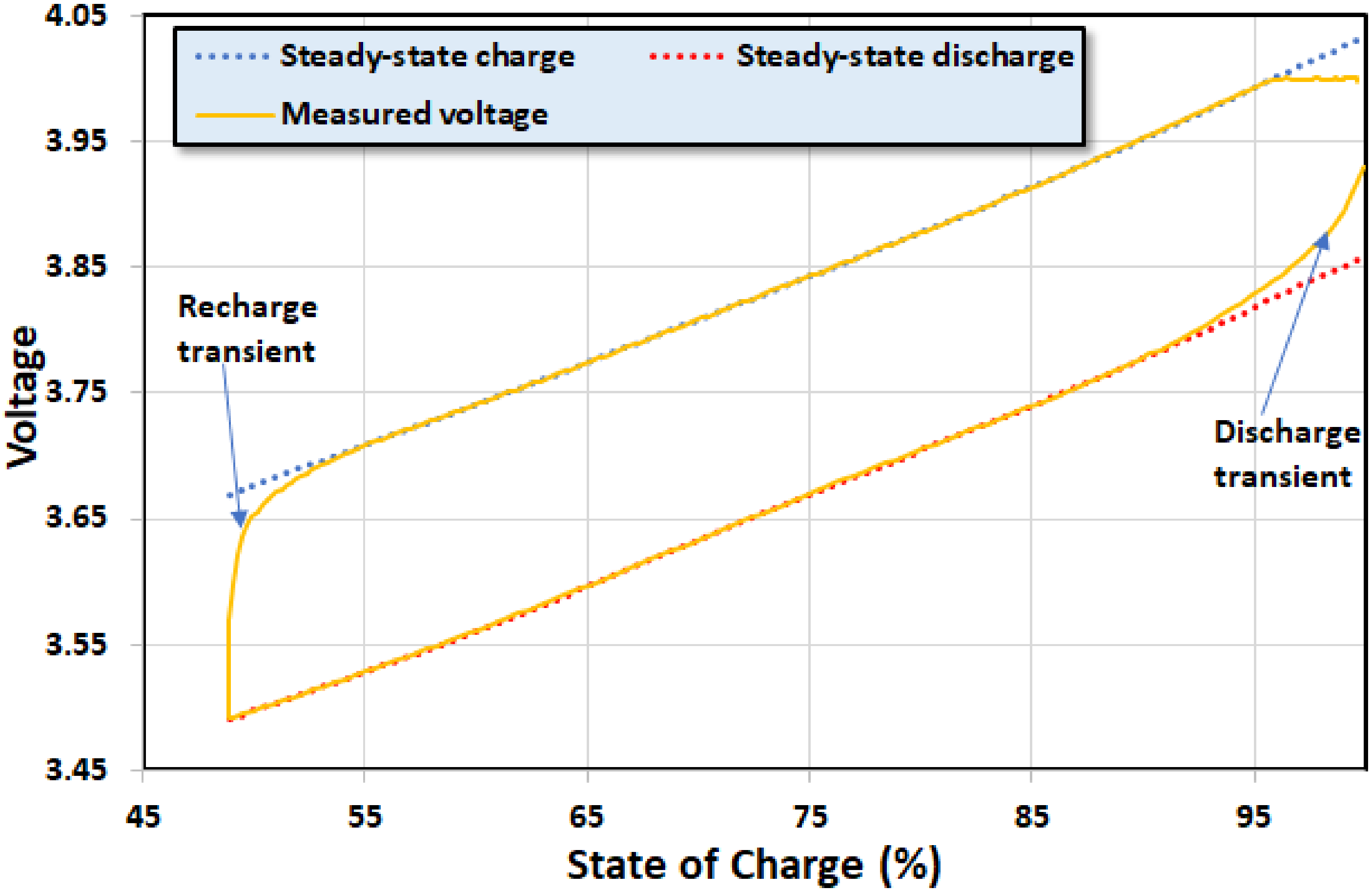
- DCR is based on steady-state charge and discharge voltage difference

- Purely ohmic resistance can be determined from the instantaneous change in voltage when the current changes
- Ohmic resistance part of, but significantly less than the DC resistance



Non-Steady-State Voltage Responses

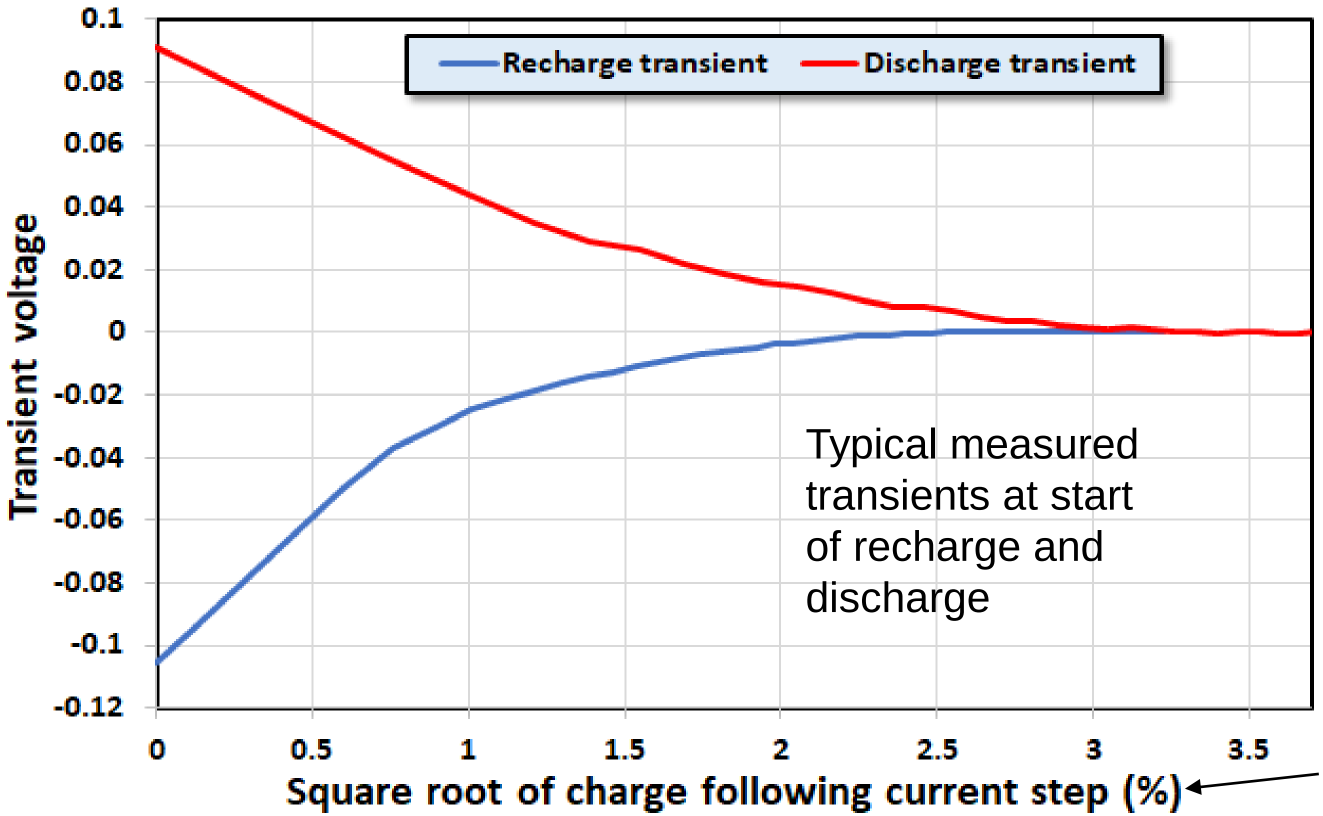
- **Voltage transients in Li-Ion cells are caused by diffusional relaxation of the lithium ion gradients in the electrodes when the current changes**



Transients are the deviation between measured voltage and steady-state voltage

Evaluation of Transient Voltage Responses

- **Diffusional response in each electrode is proportional to the square root of charge, approaching zero as a new steady state is approached**
- **Measured transients can be accurately fit to the sum of two diffusion functions. Enables diffusion kinetics to be tracked over life.**
- **Each diffusion function is described by an amplitude and an initial slope**

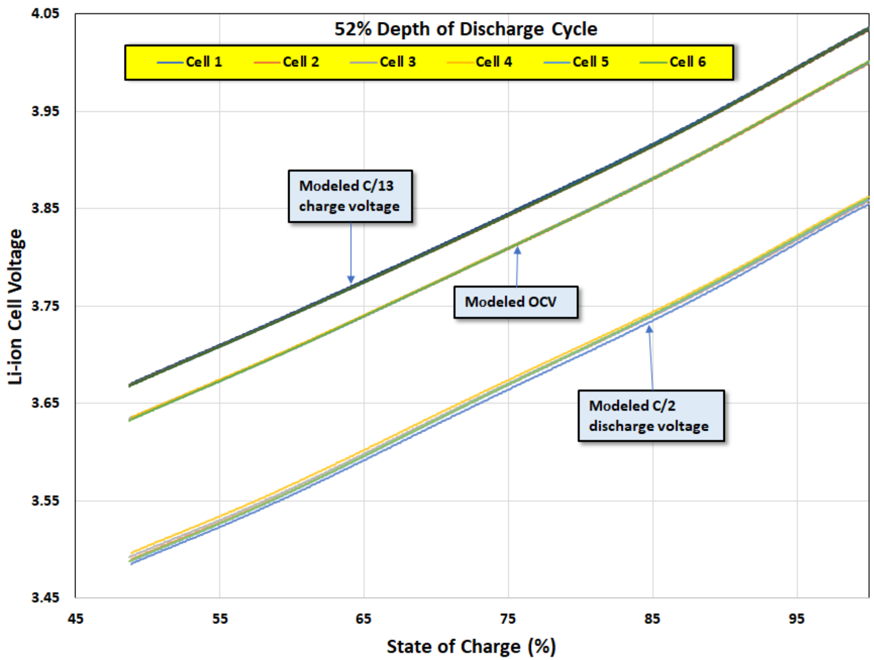


Diffusion time constants are independent of current if plotted *vs* $(\text{Charge})^{1/2}$ instead of $(\text{Time})^{1/2}$

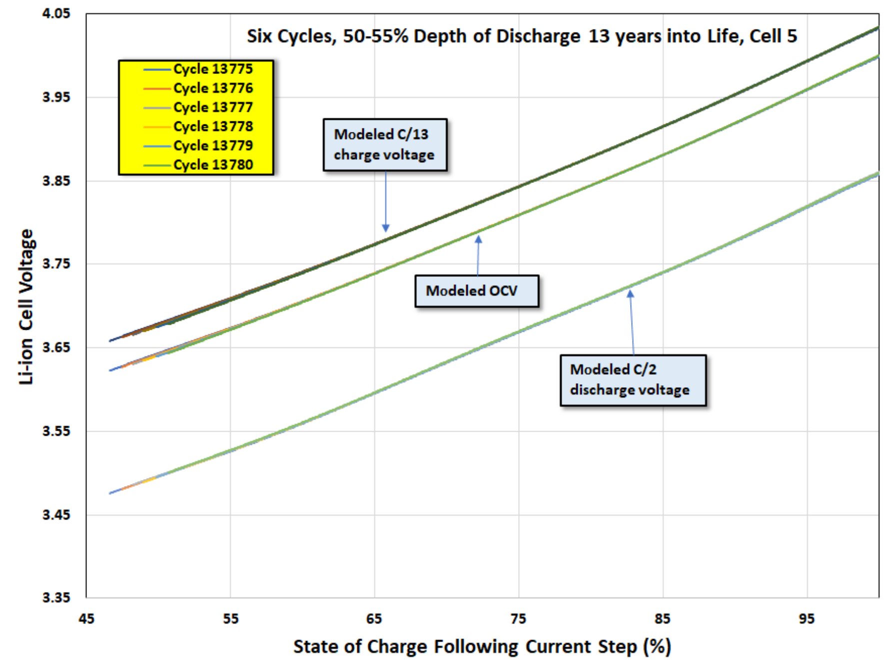
Variability of ROM Open-Circuit Voltages

- The OCVs in Reduced-Order Models generated for separate cycles or multiple cells show little variability

Six similar cells cycled together



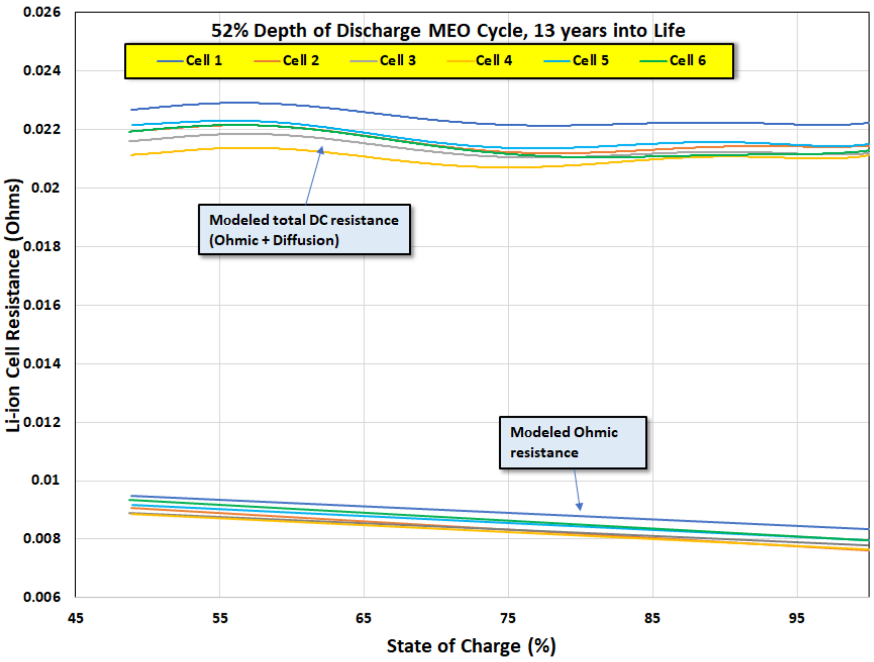
Six sequential cycles for the same cell



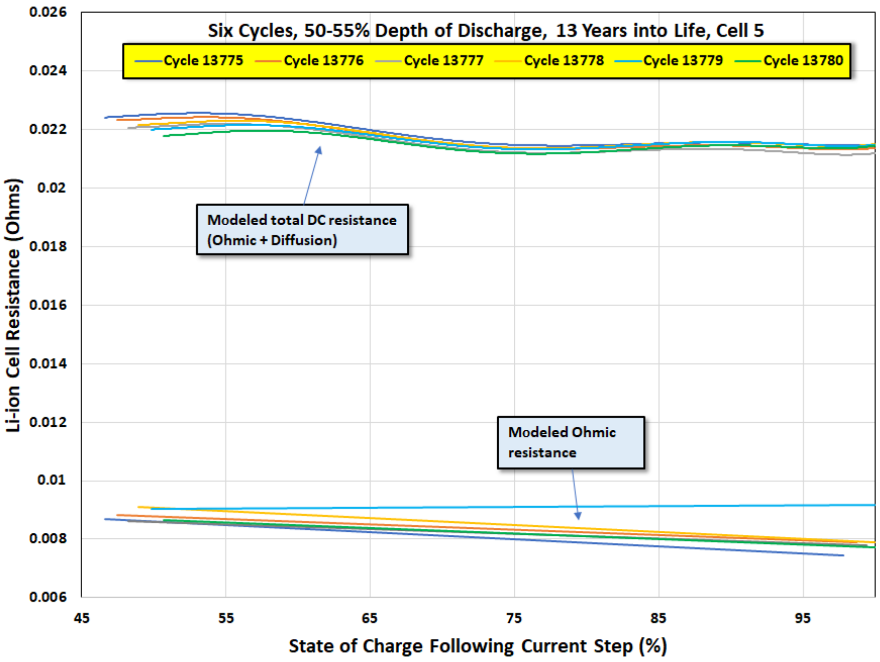
Variability of ROM DC Resistances

- The DC resistances in Reduced-Order Models generated for separate cycles or multiple cells show limited variability

Six similar cells cycled together



Six sequential cycles for the same cell

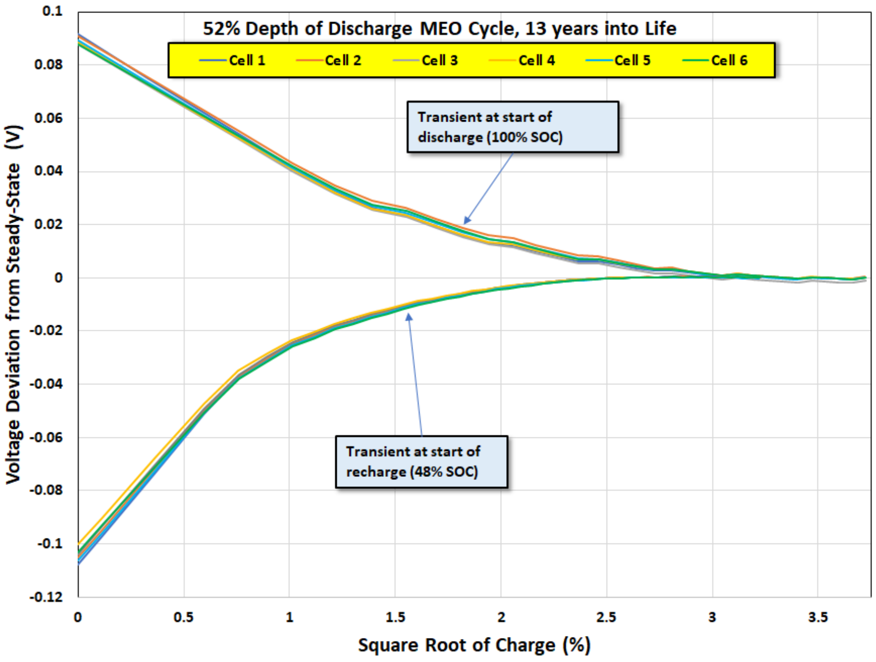


Cycle-to-cycle reproducibility should allow trending of cell variability and statistics

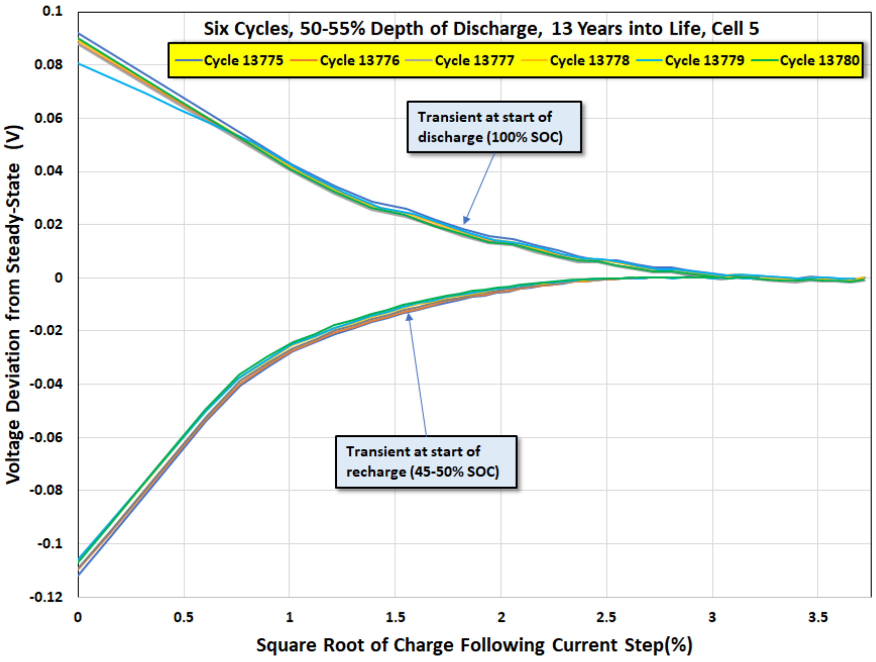
Variability of ROM Transient Response Functions

- The transient responses in Reduced-Order Models generated for separate cycles or multiple cells show some variability

Six similar cells cycled together



Six sequential cycles for the same cell



- Timing uncertainties for data taken during immediately after current transition can affect transients (see cycle 13889 above)

A machine learning algorithm can recognize anomalous behavior, and discount it

Future Plans

- **Manually analyzing cycles from a large database is <u>not</u> our path**
- **An agent will be created to autonomously scan life-test databases**
  - *For each cycle a reduced-order-model will be generated*
- **Each ROM will serve as a state-vector input to a neural net at time t**
- **The entire ROM time series will be used to train a LSTM neural net**
- **A trained neural net can be useful**
  - *Capture and help visualize all features contained within a life test*
  - *Predict likely performance into the future, and life capability*
  - *Predict performance at any point in life for untested operating profiles*
  - *Evaluate observed and expected trends*
  - *Characterize variability in cell performance and life*
  - *…and others*
- **We expect to provide an update next year**

Conclusions

- **A Reduced-Order-Model has been defined that can capture the performance behaviors of Li-ion cells**
- **Provides a physics-based framework with the flexibility to predict both steady-state and pulsed charge and discharge behavior**
- **A ROM can be quickly produced from each cycle in a long-term life test database**
- **Modern machine learning tools should be capable of "learning" the cycling behaviors which these ROMs pattern**
- **The goal of this project is to produce a neural net model that can provide Li-ion cell and battery performance over life**

Unclassified