A First Principles-based Li-Ion Battery Performance and Life Prediction Model Based on Single Particle Model Equations†

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by

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Topics

- Overview
- Single Particle Model (SPM)
- Dakota Development
- Dakota Verification, Sensitivity Studies and Validation
- Summary

Overview

- **Program Objective -** *Develop a unique object-oriented Li-Ion battery operations model,* **Dakota***, based on first principles, that describes and predicts the performance of Li-Ion cells and batteries under various operational modes and environments*
- **Why GAC and JPL? -** *GAC's object-oriented computer models of complex engineering systems. JPL's Li-Ion expertise and LEO cycling cell test data.*
- **Approach -** *Adapt SOA* "first-principles" *Single Particle Model (SPM) (Ralph White) into a cell / Battery Performance Prediction Operations Model. Verify model with LEO cycling cell test data.*
- **What's Unique? -** *Developed from first-principles Dakota utilizes techniques developed for balloon flight and other prediction models. It is highly extensible and platform independent. Engineer-friendly simulation environment. Framework for a comprehensive battery model.*

Long-term Goals for Battery Operations Model

- Simulate performance and life of a cell or battery
- Simulate changes during operation, e.g., cell or battery imbalance in series or parallel configurations
- Optimize cell / battery design and configuration
- Assess capability for a cell or battery design to meet a mission requirement
- Manage battery operation for long term success
- Assess new cell / battery technologies
- Design and size power subsystems
- Map and simulate manufacturing processes

Key Dakota Approach and Innovation

- Develop an object-oriented, desktop tool based on electrochemical first-principles, useable by system engineers. (not an esoteric Fortran code with text file configuration parameter lists)
- Incorporate simulation of individual cell charge and discharge characteristics and cycling performance
- Include simulation of orbital battery operations in LEO including thermal and mechanical interactions
- Provide a modular architecture that allows
  - A scalable user interface
  - Easy “what if” playing
  - New physics to be added now and in the future
  - Cell design parameters
  - Battery interactions with wide variety of environments

Battery Modeling Projects

Battery Modeling Projects

- **Phase II STTR with JPL - *SPM Dakota***
  - Single Particle Model (SPM) focused on LEO model development
  - Already incorporated into Dakota engine
  - Much faster than Full Physics Model (FPM)
  - Limited to low rates and nominal temperatures
  - In the prototype model development, we are extending the SPM to higher rates and a wider range of temperatures

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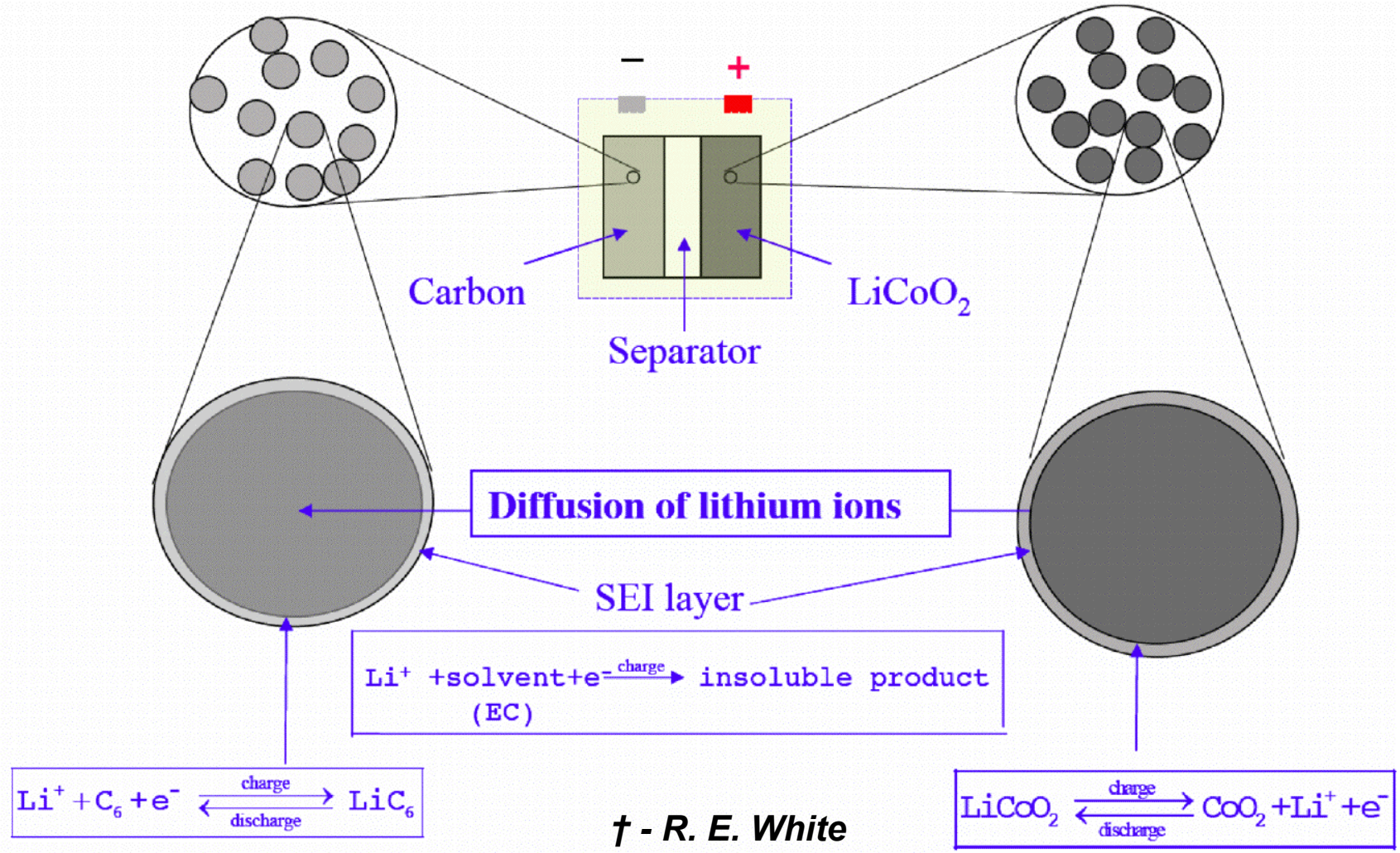
- **Phase I STTR with TTU - *RFM Dakota***
  - **Reformulated Model (RFM) focused on LEO model development**
  - **Faster than FPM and handles higher rates and a wider range of temperatures like the FPM**
  - **Higher fidelity at a cost of somewhat slower speed than SPM**
  - **In Phase I, RFM equations for three Li-Ion chemistries were incorporated into Dakota along with the LEO orbit scenario**

Project Plans

- Selected Single Particle Model (SPM) of Ralph White (USC) as our first-principles model
- In Phase I, we developed a proof-of-concept tool based on the SPM
- Focused Single Particle Model (SPM) on LEO simulation development
- Validated operational performance based on NASA/JPL test data of the prismatic Mars Exploration Rover (MER) 8-AH-rated cell from Lithion
- In the Phase II prototype tool development, we are:
  - Extending the SPM to higher rates and a wider range of temperatures
  - Incorporating environment, cell interactions and operational factors

Single Particle Model (SPM)†

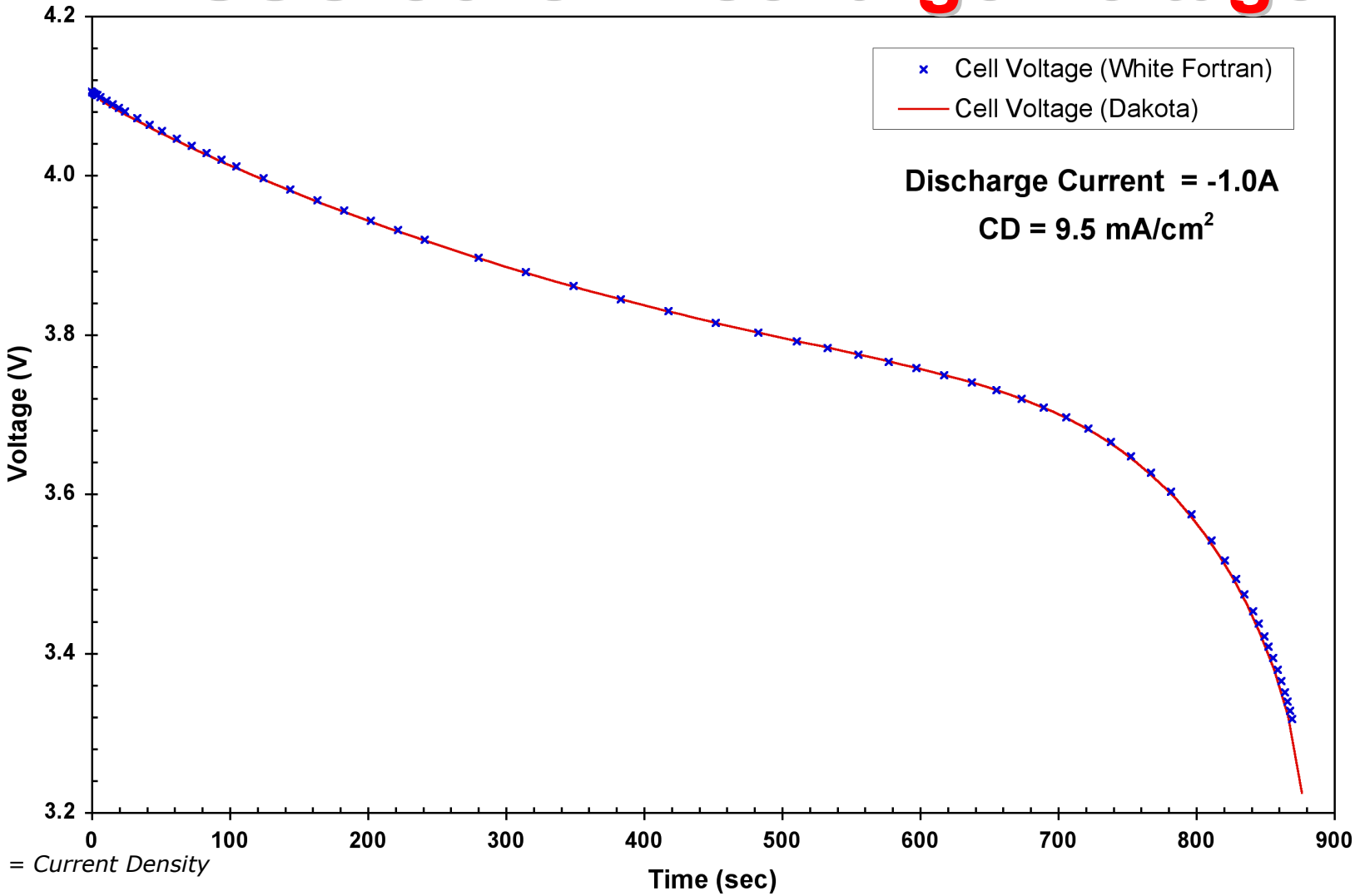


† - R. E. White

Dakota Development

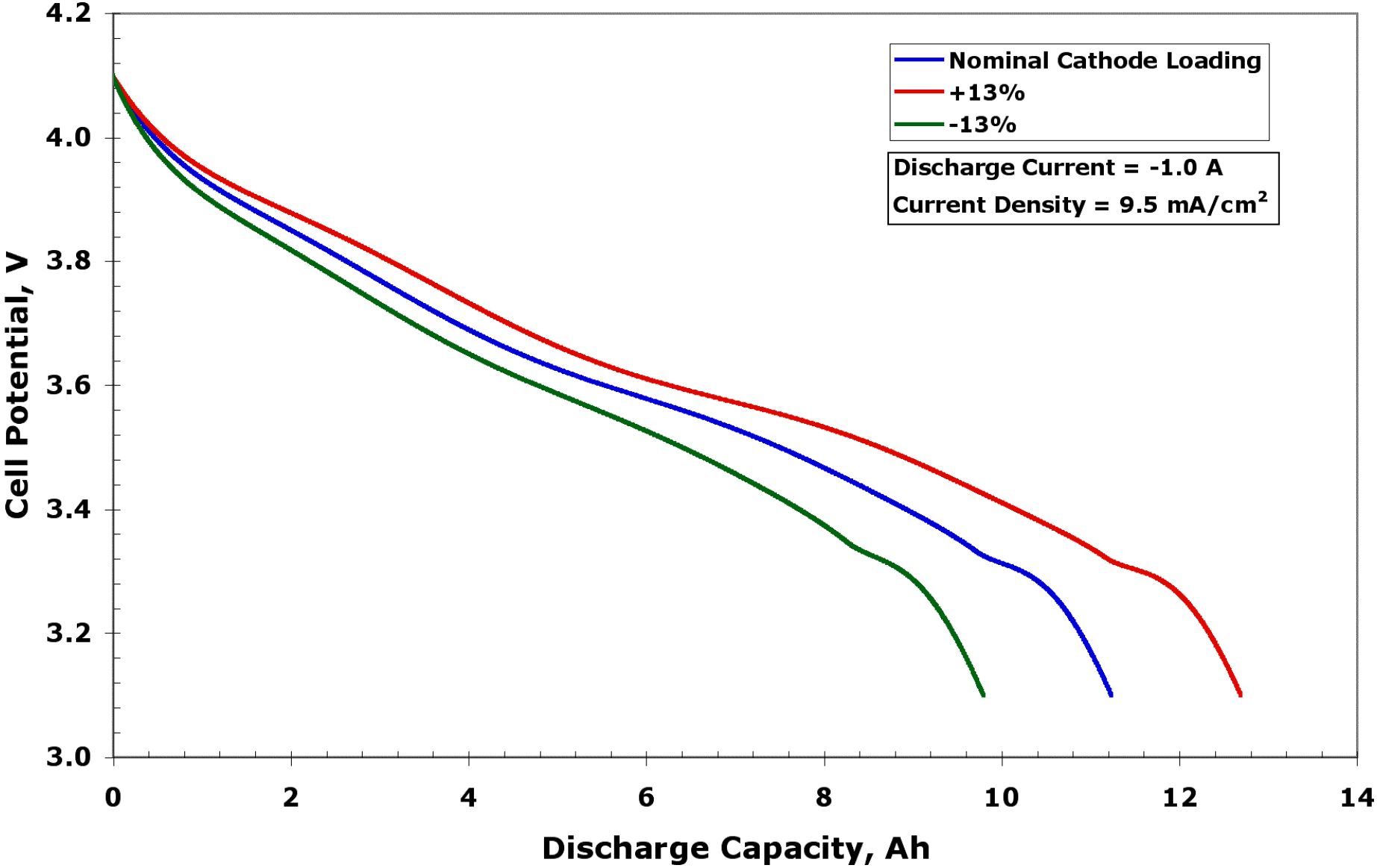
- Incorporated the SPM into the Dakota engine
- Developed a graphical user interface (GUI)
- Developed cell and battery designer wizards
- Incorporated preliminary LEO cycling protocol
- Verified Dakota code against White's SP Fortran model of USG cell design
- Carried out sensitivity studies of discharge behavior as a function of rate constants and diffusion coefficient

SPM Dakota Verification for USG Cells: Discharge Voltage



CD = Current Density

Cathode Loading Sensitivity



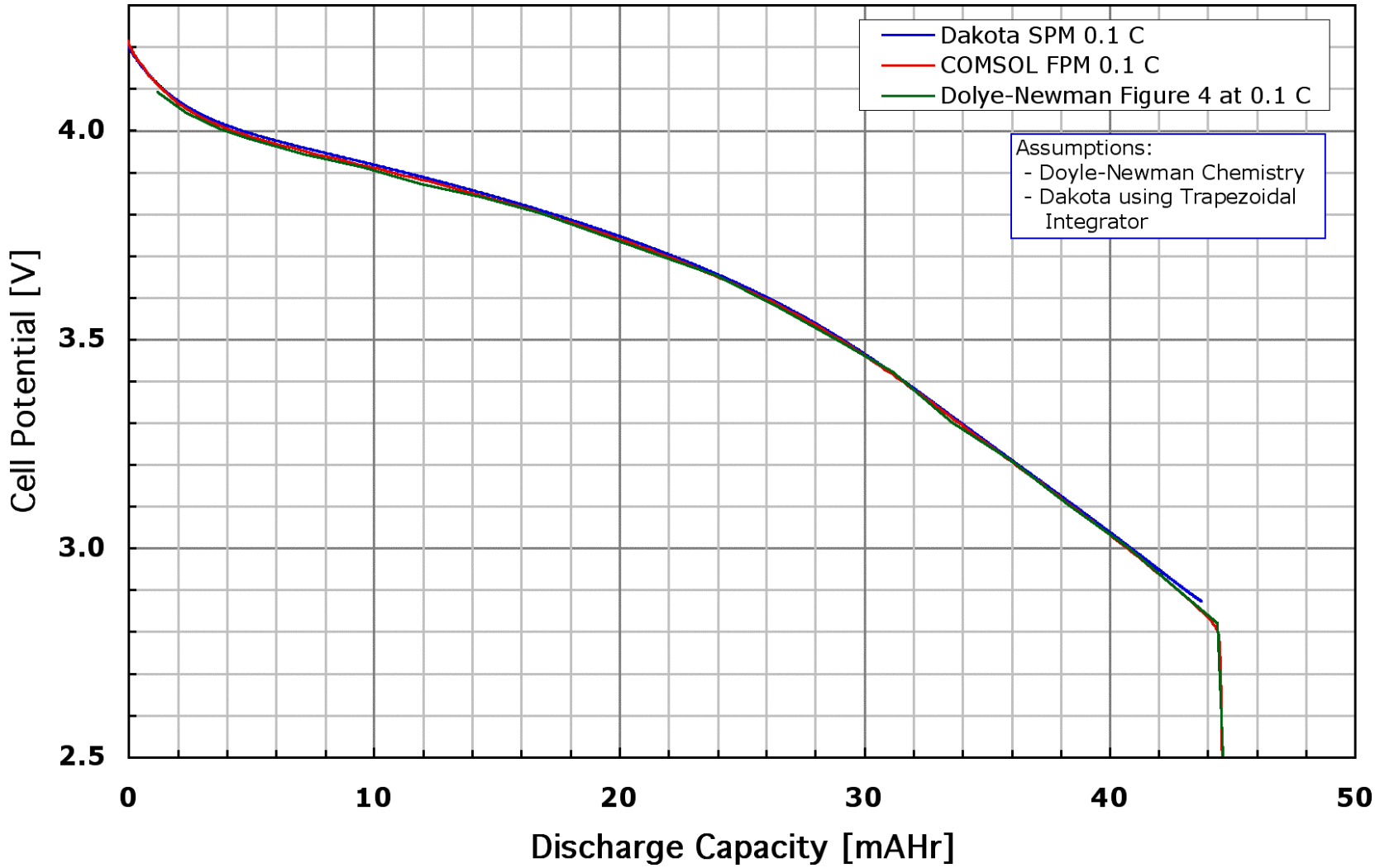
SPM Dakota Validation Strategy

- Three Chemistries
  - Doyle-Newman* (D-N) - $Li_yMn_2O_4$, Li_xC_6
  - USG - Li_xCoO_2, Li_xC_6
  - JPLY - $LiNi_xCo_{(1-x)}O_2$, Li_xC_6
- Incorporate cell chemistry and cell parameters into both JPL Dakota and a Full Physics Model (FPM)
- Validation - Compare SPM Dakota results with
  - Doyle-Newman published results
  - JPLY LEO cycling data, and
  - COMSOL full-physics model results for all three chemistries

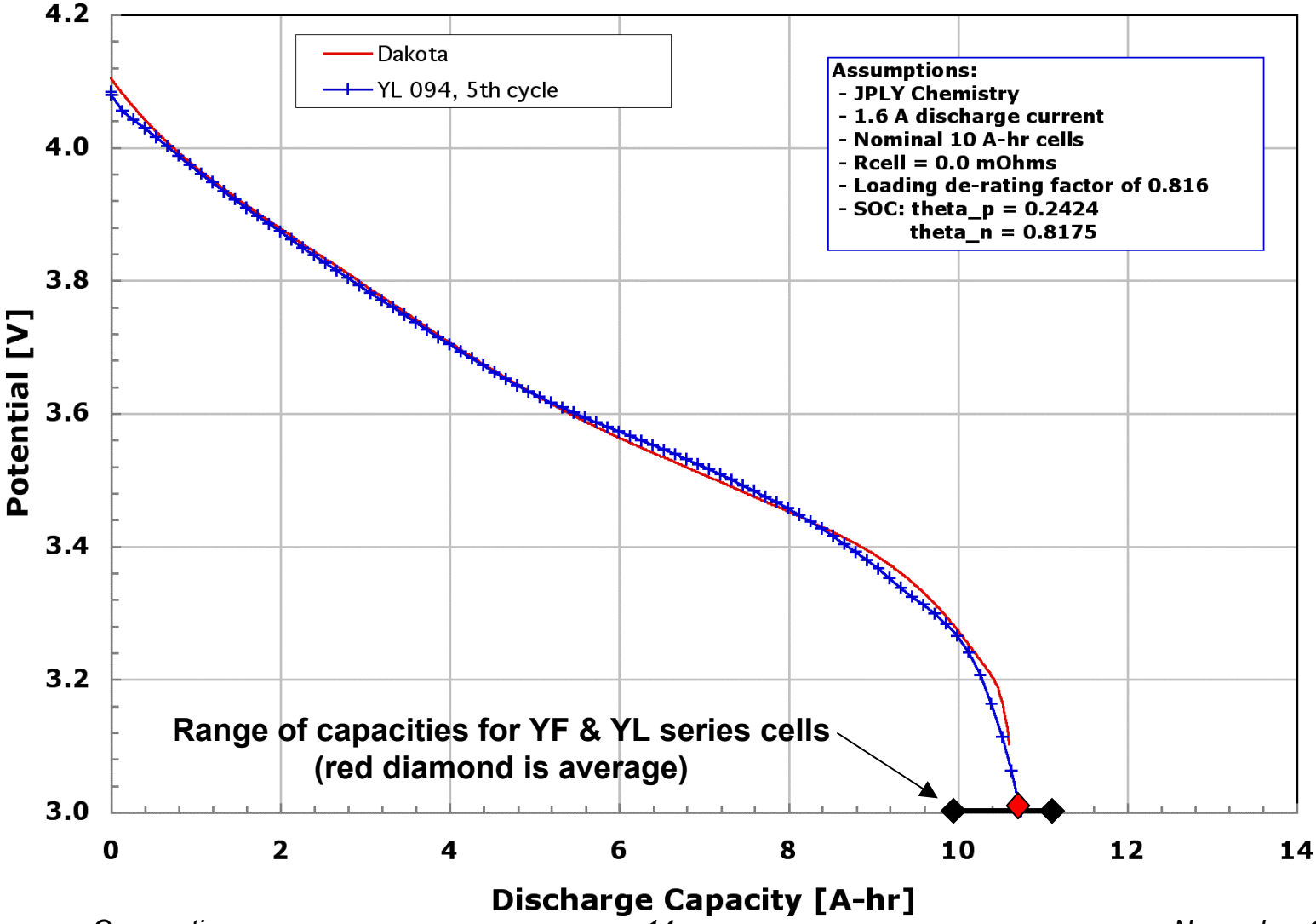
** - Doyle-Newman, et. al, Comparison of Modeling Predictions with Experimental Data from Plastic Lithium Ion Cells, J. Electrotrochemical. Soc., Vol. 143, No. 6, June 1996*

Doyle-Newman Comparison

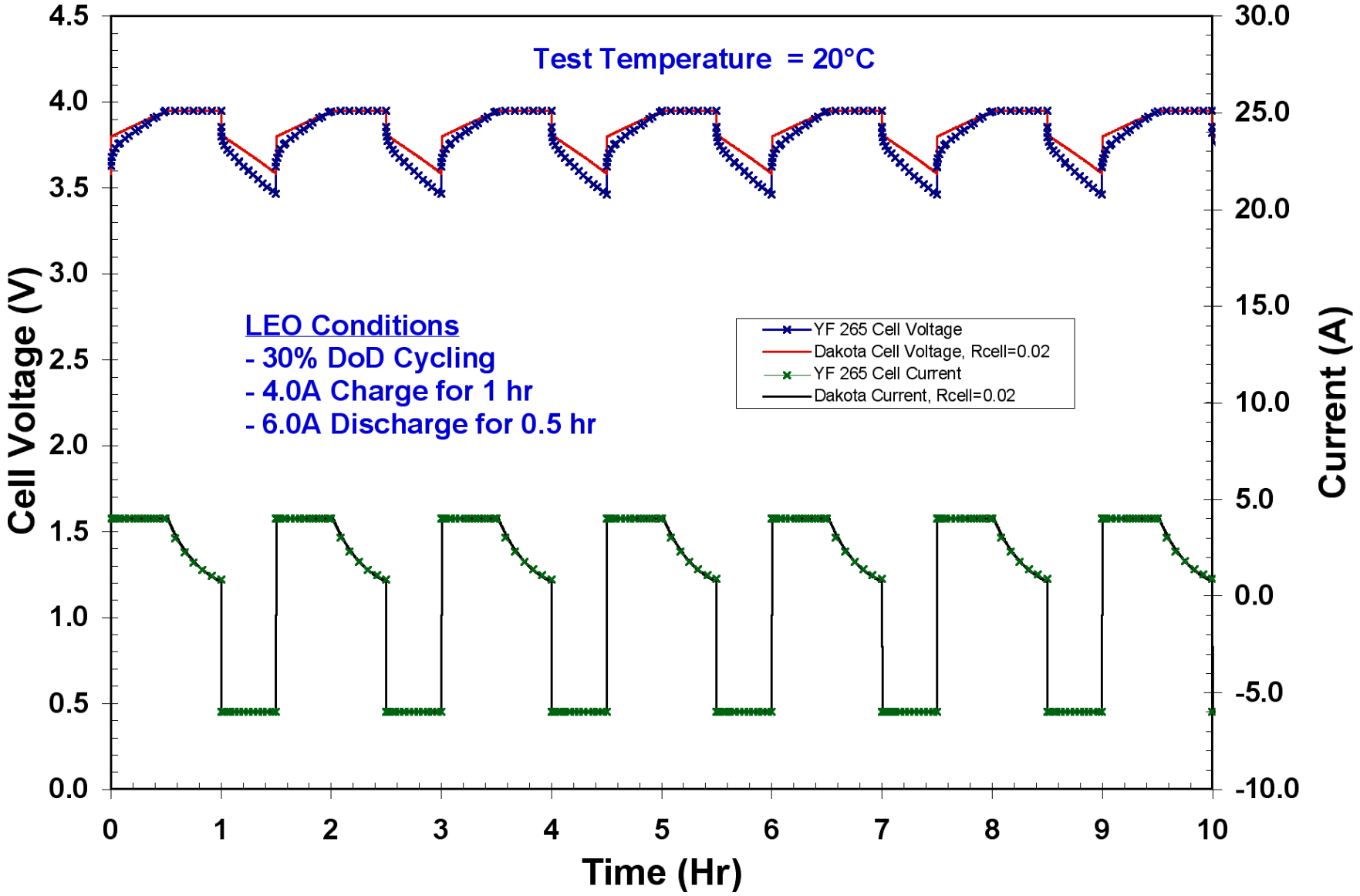
0.1 C



MER Chemistry: 100% DOD Discharge



MER Chemistry: LEO Cycling



Summary

- We have leveraged our simulation and Li-Ion cell and battery expertise to develop a unique and advanced battery operations tool to predict life and performance
- Dakota tool adapts the first-principles SPM that has been verified with White's Fortran SPM-based cell model
- Our validation data compares very favorably with JPL's test data on the MER 8-Ah-rated Li-Ion cells and published data on $Li_yMn_2O_4$, Li_xC_6 (Doyle-Newman chemistry)
- A model validation strategy has been formulated and is in the process of being implemented
- The SPM Dakota tool now can study three chemistries under LEO cycling conditions, i.e. Doyle-Newman, USG and JPL MER

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