A First Principles-based Cell and Battery Simulation and Modeling Tool

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Abstract: *Global Aerospace Corporation (GAC), along with its research partners the Jet Propulsion Laboratory (JPL) and Washington University (WU), is developing a unique computer simulation tool, "Dakota", to provide a reliable, high-fidelity method for predicting Li-Ion cell and battery operational performance and life. The development of Dakota has involved two modeling approaches. One approach is based on the Single Particle Model developed by Ralph White. The second model approach is based on the Reformulated Model of Venkat Subramanian. The basis for these approaches will be described. Dakota was validated against full physics model predictions, published results, and experimental cell cycling data. In addition, three different Li-Ion chemistries have been incorporated into Dakota and its results validated. The operational performance of the Dakota was validated based on NASA/JPL test data of the prismatic Mars Exploration Rover (MER) 8-Ah-rated cell from Lithion. Dakota operation was demonstrated for pulse discharge operation and cell cycling performance was assessed.*

Keywords: battery, Li-Ion, lithium, rechargeable lithium, battery software model, battery model, aerospace battery, battery testing.

Introduction

Global Aerospace Corporation, in collaboration with its partners, has been developing and extending its unique first-principles-based Lithium-Ion cell and battery operations model, "Dakota", into new models, chemistries and capabilities. As a desktop tool, Dakota is designed to describe and predict cell and battery performance and life under various operational modes and environments. The GAC effort to produce a first principles-based battery operations tool involves two distinct approaches being funded by the Missile Defense Agency (MDA) Small Business Technology Transfer (STTR) Program. One approach has been to incorporate the Single Particle Model (SPM) equations developed by Dr. Ralph White into Dakota (SPM Dakota), where JPL is our STTR partner. The second approach is to incorporate the Reformulated Model (RFM) equations developed by Venkat Subramanian into Dakota (RFM Dakota) and Washington University in St Louis is our STTR partner.

These object-oriented models are based on fundamental, first principles equations that describe chemical, electrochemical, and mechanical performance of cells. These first-principles models can be used in place of the more commonly used empirical models. They have the capability for providing long term performance predictions under user-specified operating conditions determined without lengthy and costly real time testing. In the Dakota battery operation model, object-oriented programming methods are used to construct software models that relate to the physical components of the battery..

Both the SPM and RFM approaches to Dakota include user defined cell and battery design parameters that provide a capability to simulate charge and discharge profiles as well as operational cycling. Dakota is designed to be an engineer-friendly, extensible and platform independent tool. As described below, these approaches have been validated against results described in the literature, full-physics model code results, or experimental cell test data. Both STTR efforts are aimed at predicting long-term battery performance in aerospace missions and can be applied to other battery related applications

Cell and Battery Models

There are a variety of types of battery prediction and performance models including empirical and mathematical.

Empirical Models: The most common battery performance model is the empirical type that is designed and developed by aerospace engineers to predict performance for their unique missions. These involve user designed real time lengthy and costly cell and battery testing, the results of which are utilized in curve fitting equations for predictions. Most if not all aerospace users have their unique empirical models.

Full Physics Model (FPM): An RFM was developed by Fuller, Doyle and Newman [1] based on the physics and chemistry of the Li-Ion cell. It is based on first principles and incorporates detailed algorithms to characterize cell physics and chemistry. It has been run on multi-physics programs, e.g. COMSOL. As expected, it is computationally intensive, which makes long-duration battery simulations impractical.

Single Particle Model (SPM): The SPM for Li-Ion chemistry was developed by Ralph White of University of South Carolina [2]. Used in the SPM Dakota battery performance model, its approach is to integrate each cell electrode into simple, single particle whose behavior can be derived from simple equations. It is fast but lower in fidelity than the FPM. Because the SPM is simplified, it is presently limited to low rates and nominal temperatures.

Reformulated Model (RFM): The RFM approach was developed by Venkat Subramanian at Washington University in St. Louis [3]. The approach used for the RFM

Dakota is to "reformulate" the full physics equations into computationally efficient algorithms. It is two orders of magnitude faster than FPM but slower than the SPM, however, it can handle higher rates and a wider range of temperatures, like the FPM. This method produces higher fidelity but tailored to a specific variable set.

The Single Particle Model (SPM)

A pictorial view of Ralph White's Single Particle Model is shown in Figure 1, where a single particle represents all particles of an electrode. The model is based on the FPM of Fuller, Doyle and Newman but makes several simplifying assumptions. These include: a) the concentration of the Lithium ions in the electrolyte is assumed to be constant across the cell sandwich, b) the potential in the solution phase is assumed to be a constant across the cell (zero volts relative to a Li/Li^+ reference electrode in the solution phase), c) the potentials in the aluminum current collector and the cathode are assumed to be the same and depend on time, not position through the electrode, d) the potentials in the anode and the copper current collector are assumed to be the same and depend on time, not on position, and e) the cell potential is given by the difference between the cathode potential and the anode potential.

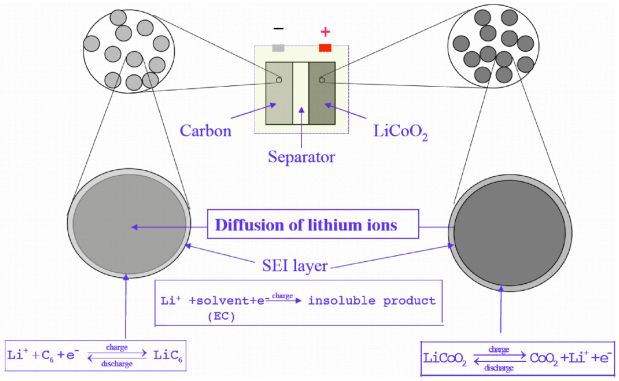

Figure 1. White Single Particle Model Schematic

SPM Dakota: The first step in the effort to produce a SPM Dakota Model was to develop a proof-of-concept tool based on White's single particle model. The initial Phase I effort was focused on predicting performance a Low Earth Orbit (LEO) simulation. The operational performance was validated based on NASA/JPL test data of the prismatic Mars Exploration Rover (MER) 8-Ah-rated cell from Lithion.

The Proof of Concept SPM Dakota contains cell and battery designer wizards and a user friendly Graphical Interface Unit (GUI). It was used to verify the Dakota code against White's SP Fortran model of the USG cell design, fix high-priority bugs, and to develop a preliminary LEO cycling protocol. The goal of the Phase II effort, is to develop a prototype tool with improved cell and battery performance and prediction fidelity, extend the SPM to higher rates and range of temperatures and incorporate environment, cell interactions and operational factors.

Model Verification and Validation: The first step in validation of the SPM Dakota was to demonstrate that the tool produced results consistent with the existing models. First the SPM Dakota matched results of the Fortran SPM generated by White. It verified the capability of the SPM Dakota model to match the charge curve of White's Fortran SPM model for USG chemistry (Li_xCoO_2,/Li_xC_6), at a current density of 9.5 ma/cm^2 (C/2). As seen in the figure, the charge curves for the two cases overlap as they should because we correctly incorporated the SPM into Dakota.

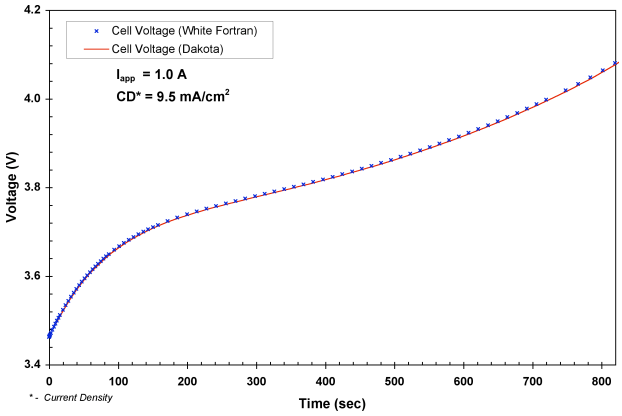

Figure 2 Verification of SPM Dakota with White's Fortran SPM code

Next the Dakota results for two chemistries were compared with published results and experimental data. The Dakota was also compared with the Full Physics Model of the Doyle-Newman (D-N) cell chemistry ($Li_yMn_2O_4/Li_xC_6$) [4] for cell discharge and with the Mars Exploration Rover (MER) 10-Ah nominal, 8-Ah-rated, cell chemistry ($LiNi_xCo_{(1-x)}O_2/Li_xC_6$) for capacity and LEO cycling. The results are shown in Figure 3 through Figure 5.

Figure 3 is a comparison of SPM Dakota and the FPM of the D-N chemistry in a small, 42-mAh polymer cell. The SPM Dakota model compared quite favorably with the RFM for the C/10 discharge result published in the D-N reference article.

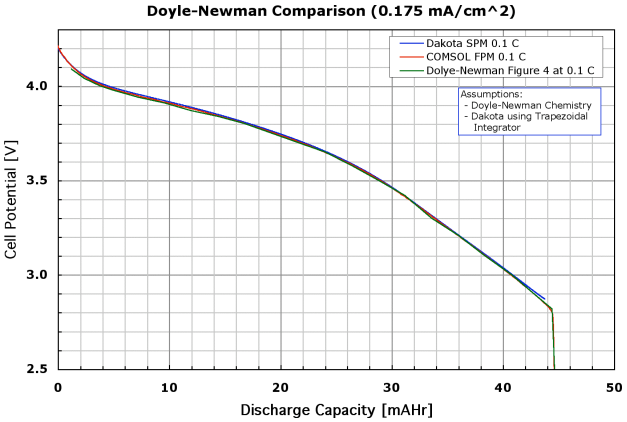

Figure 3 Comparison of SPM Dakota and RFM published results of the D-N chemistry

Figure 4 is a comparison of the SPM Dakota with actual data from a MER Li-Ion cell with the $NiCoO_2$/MCMB chemistry. A cell designated YL094, and the SPM Dakota results were compared. The discharge rate was 1.6 A, which is C/5 based on the rated capacity of this cell. The YL094 cell was selected since its capacity was at the average capacity for the YL and YF MER cells groups.

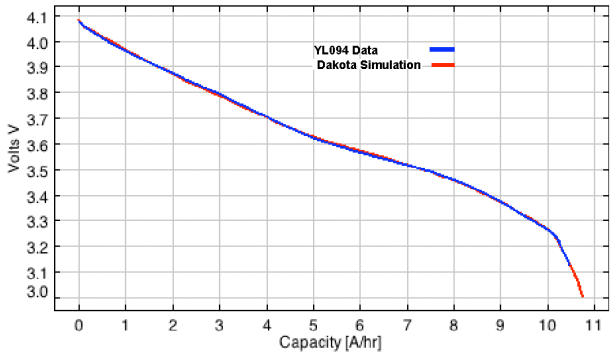

Figure 4 Comparison of SPM Dakota with JPLY (MER) Cell Chemistry at 100% DOD

A comparison of a SPM Dakota simulation and the cycling of a MER cell for a Low Earth Orbit (LEO) protocol at 20°C is shown in Figure 5. The voltage and current outputs are compared with the SPM Dakota. The protocol was 30% DOD (4A for initial charge to 3.95 V followed by taper for a total of 60 minutes and 6A discharge for 0.5 hours. The voltage comparison is shown in the top curves.

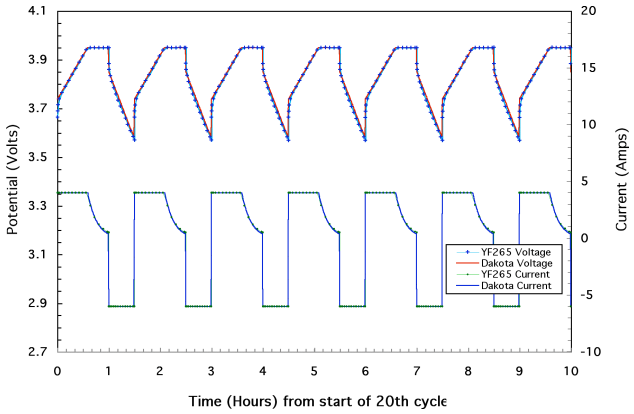

Figure 5. Comparison of a SPM Dakota simulation with a MER cell under LEO cycling

Status and Summary of SPM Dakota Effort: The SPM Dakota was validated with two chemistries, which provides confidence in the Dakota approach. Favorable comparisons were achieved with JPL's LEO cycling of MER 8-Ah-rated Li-Ion cells. Additional work is underway to extend rate and temperature envelope of the SPM.

The RFM Dakota

The goal of the RFM Dakota effort is to produce a battery performance model that has high-fidelity and that is still reasonably fast. In the Phase I of this effort a proof of concept battery tool that predicts LEO orbit battery life and performance at moderate temperatures and under a variety of operational conditions (charge, discharge, taper, and pulse-power) was developed. RFM equations for three Li-Ion chemistries were incorporated into RFM Dakota along with LEO orbit scenarios for cycling predictions under high current loads.

The Reformulated Model Concept: This reformulation approach developed by Subramanian et al. [3] involves starting with the partial differential equations of the D-N FPM. A typical FPM has 5000 states. A RFM can have less than 50 state variables after reformulation. Figure 6 shows an overview of the reformulation process.

The RFM is based on the porous electrode theory. The multi-equation output (27 or more) from the reformulation process predicts battery behavior without compromising accuracy and physics. It can be applied to both charge and discharge processes. Two initial sets of RFM equations were incorporated and tested in the RFM Dakota: Mn_2O_4 (D-N) chemistry and $NiCoO_2$ chemistry.

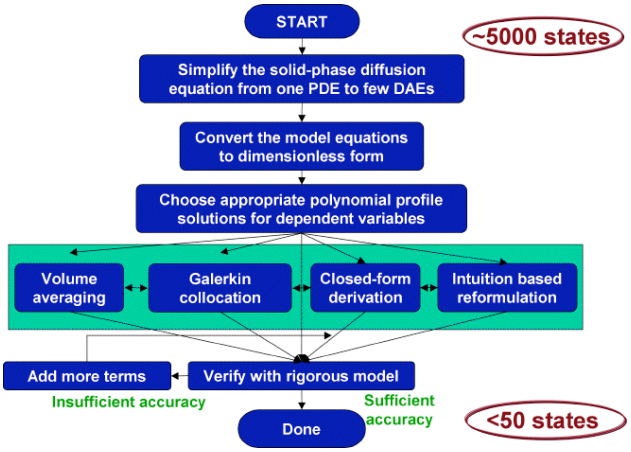

Figure 6. Overview of the Reformulation Process

RFM Dakota predictions of cycling and pulse operation: To demonstrate cycling capability and impact of a pulse using the RFM Dakota Model, a scenario was identified that would simulate the effect of the pulse charging on cell voltage and current cycling.

The scenario was to simulate a 28 day repetitive "monthly" period (14 orbits / day), 100 minute orbit normal charge to 4.1 V followed by taper. The cell would be subjected to a pulse once each day (during the middle of cycle 7 discharge), for 0.5 min at one of 3 rates. In addition, once each month during the cycle 14th discharge on the 28th day the cell would be discharged for 10 minutes at one of the 3 rates. Each scenario is compared with no pulse cycling. Figure 7 is a schematic of the pulse discharge scenario.

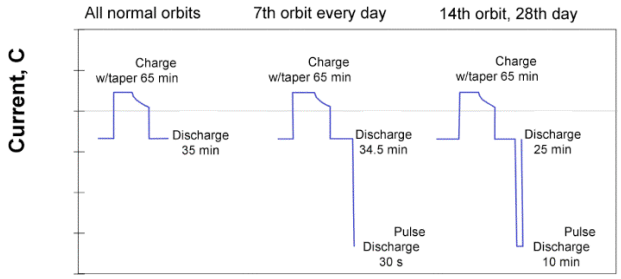

Figure 7. Pulse cycling regime scenario

Figure 8 and Figure 9 demonstrate how the time to return to full charge and normal taper is affected by the discharge pulses. The current profiles for the scenario are shown in Figure 8. The lowest pulse has little effect since the current profile returns to the full charge profile within 1 cycle. After the mid-level pulse, the voltage returns to normal on the 3rd cycle and after the highest pulse the current returns to normal full charge on the 6th cycle. On the right of the figures the effect of the short, 0.5-minute pulse is shown. The current returns to normal after the 1st cycle after all pulses.

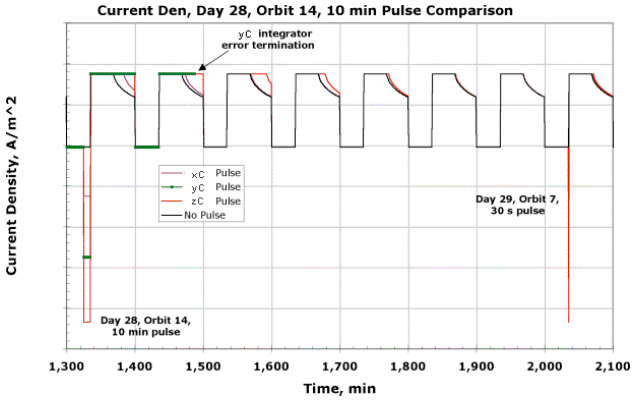

Figure 8 Dakota comparison of cell current density with and without pulse cycling

The curves demonstrate a similar sequence in the voltage profiles in Figure 9. In the case of charge current it is noted that with the highest pulse the voltage fails to return to the max voltage limit of 4.1 volts until the third cycle and then only for a short time until the 6th cycle when it returns to the normal pattern.

Status and Summary of the RFM Dakota Effort: RFM Dakota has been validated with multiple chemistries that has provided confidence in this approach. A proof-of-concept set of RFM equations for D-N chemistry was incorporated into Dakota and its results verified. A pulse power cycling regime was simulated for D-N chemistry and results compared with no-pulse operation. Phase II plans are to include improved integrators/solvers and incorporate a thermal model as well as new chemistries in addition to expanding software flexibility

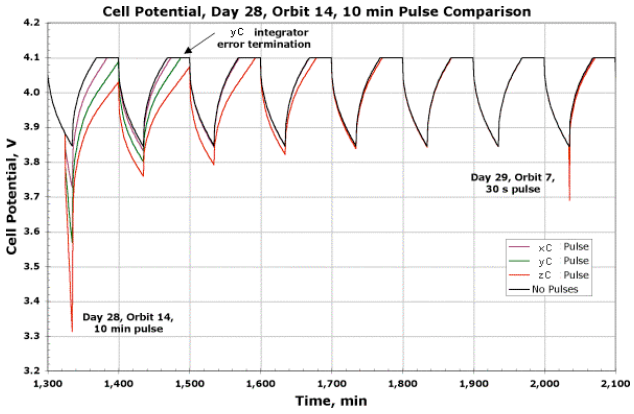

Figure 9. Dakota comparison of cell potential with and without pulse cycling

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