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

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by

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Topics

• Overview
• Reformulated Model (RFM)
• Initial Set of RFM Equations
• Proof-of-Concept RFM Equations
• LEO Pulse Cycling Regime
• Summary
Overview

• **Program Objective** - Develop a unique object-oriented Li-Ion battery model for analyzing satellite operations scenarios, 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 TTU?** - GAC’s object-oriented computer models of complex engineering systems. TTU’s Li-Ion reformulated model (RFM) expertise and experience.

• **Approach** - Adapt reformulated, first-principle, cell model to an object-oriented cell/battery operations model. Verify model with LEO cycling cell test data.

• **What’s Unique?** - 1. RFM fastest algorithm (as of today in the literature) developed from first-principles cell model. 2. Use of object-oriented code that is highly extensible and platform independent. 3. Engineer-friendly simulation environment. 4. 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

• 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

• 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
Li-Ion Battery Model for Satellite Orbit Operations Scenarios

Project Plans

• Selected the reformulated model (RFM) approach of Dr. Venkat R. Subramanian who was at TTU, now at Wash U.
• The initial objective was to develop a proof-of-concept RFM battery operations tool for a candidate Li-Ion cell chemistry focused initially on LEO Operations
• The RFM equations for two Li-Ion chemistries were incorporated into Dakota along with a simple LEO battery operations scenario
• Validated the RFM Dakota tool results against TTU-generated charge / discharge behavior data
• Simulated three different pulse charge battery operations scenarios
• Compared pulse cycling case with no-pulse operation
Li-Ion Battery Model for Satellite Orbit Operations Scenarios

START

Simplify the solid-phase diffusion equation from one PDE to few DAEs

Convert the model equations to dimensionless form

Choose appropriate polynomial profile solutions for dependent variables

Volume averaging
Galerkin collocation
Closed-form derivation
Intuition based reformulation

Add more terms
Verify with rigorous model

Insufficient accuracy
Sufficient accuracy

Done

~5000 states
<50 states

[ V.R. Subramanian+ ESL 2007 ]
Li-Ion Battery Model for Satellite Orbit Operations Scenarios

Initial Set of RFM Equations

• Two chemistries
  – Doyle-Newman Cell Model (LiMn$_2$O$_4$)
  – TTU / USG Cell Model (LiNi$_{0.8}$Co$_{0.15}$Al$_{0.05}$O$_2$)

• Characteristics of test set of equations
  – Discharge curves and dependent variables (electrolyte concentration, potential, solid-phase potential, solid-phase concentration) at $x = 0$.
  – Fixed current rate
  – Variable: State-of-charge and cutoff potential
# Li-Ion Battery Model for Satellite Orbit Operations Scenarios

## Doyle-Newman Full-Physics Model

<table>
<thead>
<tr>
<th>Region</th>
<th>Eq. No.</th>
<th>Governing equations</th>
<th>Boundary conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Positive electrode</td>
<td>1</td>
<td>( \varepsilon_0 \frac{\partial c}{\partial t} = D_{eff} \frac{\partial^2 c}{\partial x^2} + a_p (1-t_s) j_p ) initial condition ( c</td>
<td>_{t=0} = c_0 )</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>(-\sigma_{eff} \frac{\partial \Phi_1}{\partial x} - \kappa_{eff} \frac{\partial \Phi_2}{\partial x} + 2 \frac{\kappa_{eff} RT}{F} (1-t_s) \frac{\partial \ln c}{\partial x} = I )</td>
<td>(-\kappa_{eff} \left. \frac{\partial \Phi_1}{\partial x} \right</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>( \sigma_{eff} \frac{\partial \Phi_1}{\partial x} = a_p F_j )</td>
<td>( \left. \frac{\partial \Phi_1}{\partial x} \right</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>( \frac{d}{dt} c_s^{ave} + \frac{3 j_p}{R_p} = 0 ) and ( \frac{D_{L,p}}{R_p} (c_s^{surf} - c_s^{ave}) = -\frac{j_p}{5} )</td>
<td>( c_s^{ave}</td>
</tr>
<tr>
<td>Separator</td>
<td>5</td>
<td>( \varepsilon_s \frac{\partial c}{\partial t} = D_{eff} \frac{\partial^2 c}{\partial x^2} )</td>
<td>(-D_{eff} \left. \frac{\partial c}{\partial x} \right</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>( I = -\kappa_{eff} \frac{\partial \Phi_2}{\partial x} + 2 \frac{\kappa_{eff} RT}{F} (1-t_s) \frac{\partial \ln c}{\partial x} )</td>
<td>(-\kappa_{eff} \left. \frac{\partial \Phi_2}{\partial x} \right</td>
</tr>
<tr>
<td>Negative electrode</td>
<td>7</td>
<td>( \varepsilon_0 \frac{\partial c}{\partial t} = D_{eff} \frac{\partial^2 c}{\partial x^2} + a_n (1-t_s) j_n ) initial condition ( c</td>
<td>_{t=0} = c_0 )</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>(-\sigma_{eff} \frac{\partial \Phi_1}{\partial x} - \kappa_{eff} \frac{\partial \Phi_2}{\partial x} + 2 \frac{\kappa_{eff} RT}{F} (1-t_s) \frac{\partial \ln c}{\partial x} = I )</td>
<td>(-\kappa_{eff} \left. \frac{\partial \Phi_2}{\partial x} \right</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>( \sigma_{eff} \frac{\partial \Phi_1}{\partial x} = a_n F_j )</td>
<td>(-\sigma_{eff} \left. \frac{\partial \Phi_1}{\partial x} \right</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>( \frac{d}{dt} c_s^{ave} + \frac{3 j_n}{R_n} = 0 ) and ( \frac{D_{L,n}}{R_n} (c_s^{surf} - c_s^{ave}) = -\frac{j_n}{5} )</td>
<td>( c_s^{ave}</td>
</tr>
</tbody>
</table>
Li-Ion Battery Model for Satellite Orbit Operations Scenarios

Doyle-Newman

RFM Equations*

\[
c_g = YPRIME1 = -0.360988287612180473519614325667e0 \times Y11 + \]
\[
0.191473721423663165685371039105e1 \times Y2 + \]
\[
0.146117687123876805835205638937e1 \times Y3 + \]
\[
0.818581995016529393932356313404e0 \times Y4 - \]
\[
0.4407324252204205964432425294418e-1 \times Y12 - \]
\[
0.7196978672843059541344330075150e-2 \times Y13 - \]
\[
0.685083539666203007516357670348e-4 \times Y27 + \]
\[
0.97844959995730070477421151524e-3 \times Y17 + \]
\[
0.276798199212208598538807863935e-2 \times Y16 + \]
\[
0.581291671447654875471851298803e-2 \times Y15 - \]
\[
0.112100335291330779227032034152e-2 \times Y26; \]
\[\]
\[
c_g0 = YPRIME2 = -0.10473424936094342981939099480e3 \times Y11 + \]
\[
0.1046566721295686646012611750174e4 \times Y2 + \]
\[
0.103798289326955751327984326349e4 \times Y3 + \]
\[
0.71867584173894273423982899829e3 \times Y4 - \]
\[
0.5026288862439300239490175953060e2 \times Y12 - \]
\[
0.188679196717988074563774446292e2 \times Y13 - \]
\[
0.893992957759775113797091423114e2 \times Y15 + \]
\[
0.3739794328538790404048243999827e1 \times Y27 - \]
\[
0.12718542057778699829649815127e2 \times Y17 - \]
\[
0.410247122066572230038398906012e2 \times Y16 - \]
\[
0.701132161249252879771610214910e1 \times Y26; \]
\[
\]
* - Two of the shortest equations shown for illustration
Li-Ion Battery Model for Satellite Orbit Operations Scenarios

Doyle-Newman Chemistry

Dakota assumptions:
- Trapezoidal Integrator
- Time step = 0.01 (dimensionless)
- Solver tolerance = 1e-6
- Maximum solver iterations = 1000
Li-Ion Battery Model for Satellite Orbit Operations Scenarios

TTU / USG Chemistry

![Graph showing cell potential over time with two curves representing TTU Fortran and Dakota.]
Proof-of-Concept
RFM Equations

- Doyle-Newman Cell Model (LiMn$_2$O$_4$)
- Charge and discharge capability
- Taper charging
- Include enough variables to enable:
  - Initial validation of Dakota using TTU data
  - Simulating a cell according to an example cell cycling regime
  - Variables include:
    - Variable current rates up to 2C
    - Variable state-of-charge, starting and cutoff potentials
Li-Ion Battery Model for Satellite Orbit Operations Scenarios

Example Cycling Regime Assumptions

- 28 day repeating “monthly” period
- 1400 min “day”
- 14 orbits per day
- 100 min orbit period
- 35 min normal discharge
- 65 min normal charge (4.1 V taper)
- Pulse cycle scenarios
  - Once each day (during the middle of cycle 7 discharge), pulse discharge for 0.5 min at xC, yC, or zC and
  - Once each month pulse discharge for 10 minutes (During cycle 14 discharge on the 14th day) at xC, yC, or zC
Cycling Regime Schematic

All normal orbits
- Charge w/taper 65 min
- Discharge 35 min

7th orbit every day
- Charge w/taper 65 min
- Discharge 34.5 min
- Pulse Discharge 30 s

14th orbit, 28th day
- Charge w/taper 65 min
- Discharge 25 min
- Pulse Discharge 10 min
Li-Ion Battery Model for Satellite Orbit Operations Scenarios

Pulse and No-pulse Comparison: Current Density

Current Den, Day 28, Orbit 14, 10 min Pulse Comparison

- xC Pulse
- yC Pulse
- zC Pulse
- No Pulse

Day 29, Orbit 7, 30 s pulse

Day 28, Orbit 14, 10 min pulse
Pulse and No-pulse Comparison: Cell Potential

Cell Potential, Day 28, Orbit 14, 10 min Pulse Comparison

Day 29, Orbit 7, 30 s pulse
Day 28, Orbit 14, 10 min pulse
Summary

- We have leveraged our extensive modeling and Li-Ion cell and battery expertise to develop a unique and advanced battery operations tool to predict life and performance.
- The initial effort was aimed incorporating test set of 27 RFM equations for Doyle-Newman and TTU / USG chemistries and its results were verified with TTU Fortran/Maple results.
- A proof-of-concept (POC) set of RFM equations for Doyle-Newman chemistry was incorporated into Dakota and its results verified.
- A pulse power cycling regime was simulated for the POC Doyle-Newman chemistry and results compared with no-pulse operation.
- The RFM Dakota tool now can study two chemistries under LEO cycling conditions, i.e. Doyle-Newman and TTU / USG.
- In Phase II we propose to incorporate additional chemistries and a cell thermal model, explore degradation mechanisms, and improve the software flexibility and operability.
Acknowledgement

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