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

NASA Battery Workshop

Huntsville, Alabama
November 17-19, 2009

by

Gerald Halpert[1], Venkat R. Subramanian[2], Matthew K. Heun[1], Kumar Bugga[3], and Kerry T. Nock[1]

[1] Global Aerospace Corporation, 711 West Woodbury Road,Suite H, Altadena, CA 91001
[2] Now at Washington University, 1 Brookings Drive, St. Louis, MO 63130
[3] Consultant

† - This work was funded by the Missile Defense Agency Small Business Technology Transfer Program under Contract HQ0006-09-C-7073 . Approved for public release; distribution is unlimited. Approved for Public Release: 09-MDA-4976 (19 NOV 09).

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

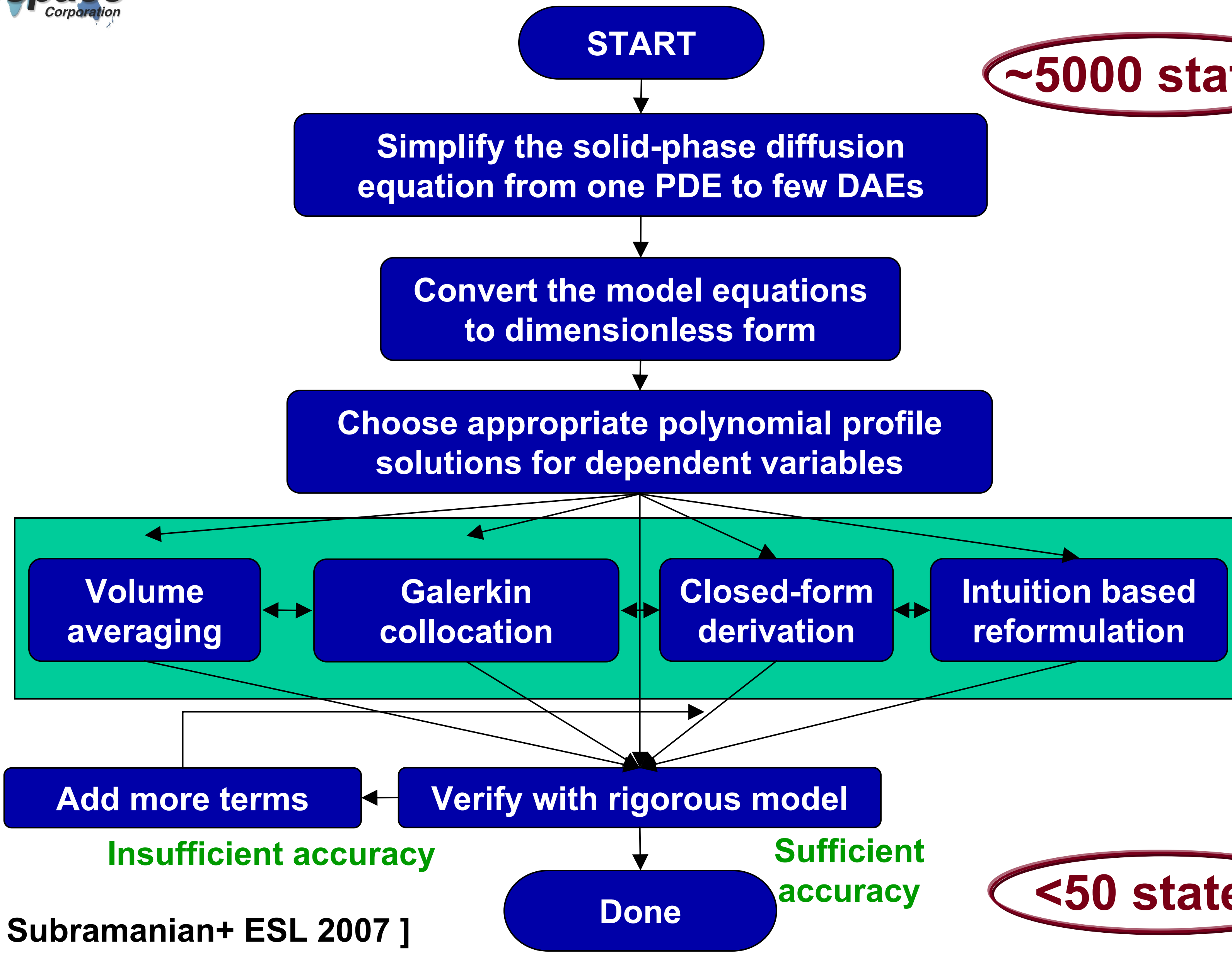
- Phase II STTR with JPL - *SPM Dakota*
  - Single Particle Model (SPM) focused on LEO model development
  - Already incorporated into Dakota engine
  - Much faster than Full Physics Model (FPM)
  - Limited to low rates and nominal temperatures
  - In the prototype model development, we are extending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

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

~5000 states



<50 states

[V.R. Subramanian+ ESL 2007]

Initial Set of RFM Equations

- Two chemistries
  - Doyle-Newman Cell Model ($LiMn_2O_4$)
  - 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

Doyle-Newman Full-Physics Model

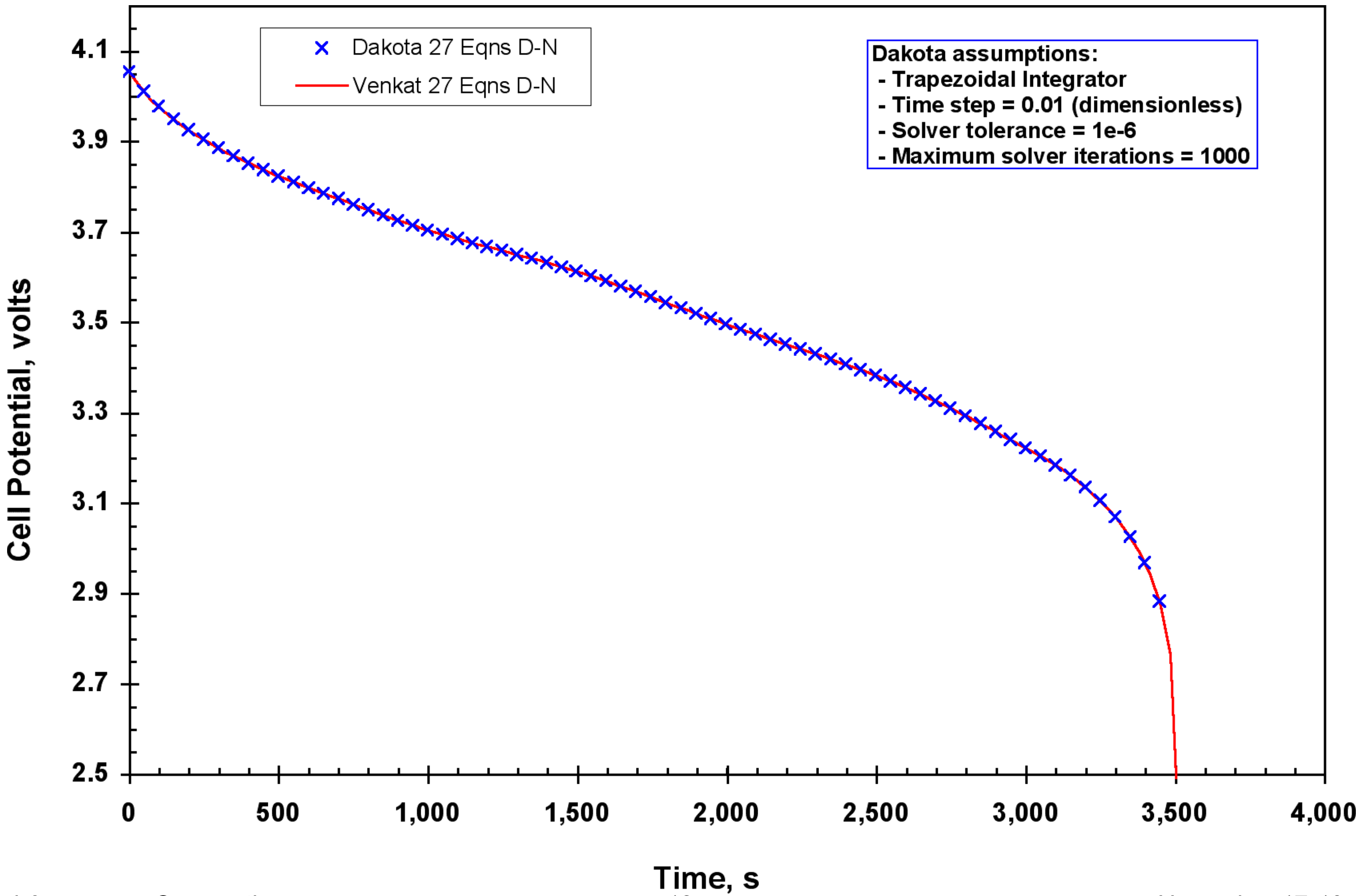
Region	Eq. No.	Governing equations	Boundary conditions
Positive electrode	1	$\varepsilon_{\mathrm{p}} \frac{\partial c}{\partial t} = D_{\mathrm{eff,p}} \frac{\partial^2 c}{\partial x^2} + a_{\mathrm{p}}(1-t_+) j_{\mathrm{p}}$ initial condition $c\big\vert_{t=0} = c_0$	$-D_{\mathrm{eff,p}} \frac{\partial c}{\partial x}\Big\vert_{x=0} = 0$ & $-D_{\mathrm{eff,p}} \frac{\partial c}{\partial x}\Big\vert_{x=l_p,-} = -D_{\mathrm{eff,s}} \frac{\partial c}{\partial x}\Big\vert_{x=l_{\mathrm{p}},+}$
	2	$-\sigma_{\mathrm{eff,p}} \frac{\partial \Phi_1}{\partial x} - \kappa_{\mathrm{eff,p}} \frac{\partial \Phi_2}{\partial x} + \frac{2\kappa_{\mathrm{eff,p}} RT}{F}(1-t_+)\frac{\partial \ln c}{\partial x} = I$	$-\kappa_{\mathrm{eff,p}} \frac{\partial \Phi_2}{\partial x}\Big\vert_{x=0} = 0$ & $-\kappa_{\mathrm{eff,p}} \frac{\partial \Phi_2}{\partial x}\Big\vert_{x=l_{\mathrm{p}},-} = -\kappa_{\mathrm{eff,s}} \frac{\partial \Phi_2}{\partial x}\Big\vert_{x=l_{\mathrm{p}},+}$
	3	$\sigma_{\mathrm{eff,p}} \frac{\partial^2 \Phi_1}{\partial x^2} = a_{\mathrm{p}} F j_{\mathrm{p}}$	$\frac{\partial \Phi_1}{\partial x}\Big\vert_{x=0} = -\frac{I}{\sigma_{\mathrm{eff,p}}}$ & $-\sigma_{\mathrm{eff,p}} \frac{\partial \Phi_1}{\partial x}\Big\vert_{x=l_{\mathrm{p}}} = 0$
	4	$\frac{d}{dt} c_s^{ave} + 3\frac{j_p}{R_p} = 0$ *and* $\frac{D_{s,p}}{R_p}\left(c_s^{surf} - c_s^{ave}\right) = -\frac{j_p}{5}$	$c_s^{ave}\big\vert_{t=0} = c_{s,\max,p}$
Separator	5	$\varepsilon_{\mathrm{s}} \frac{\partial c}{\partial t} = D_{\mathrm{eff,s}} \frac{\partial^2 c}{\partial x^2}$	$-D_{\mathrm{eff,p}} \frac{\partial c}{\partial x}\Big\vert_{x=l_{\mathrm{p}},-} = -D_{\mathrm{eff,s}} \frac{\partial c}{\partial x}\Big\vert_{x=l_{\mathrm{p}},+}$ & $-D_{\mathrm{eff,s}} \frac{\partial c}{\partial x}\Big\vert_{x=l_{\mathrm{p}}+l_s,-} = -D_{\mathrm{eff,n}} \frac{\partial c}{\partial x}\Big\vert_{x=l_{\mathrm{p}}+l_s,+}$
	6	$I = -\kappa_{\mathrm{eff,s}} \frac{\partial \Phi_2}{\partial x} + \frac{2\kappa_{\mathrm{eff,s}} RT}{F}(1-t_+)\frac{\partial \ln c}{\partial x}$	$-\kappa_{\mathrm{eff,p}} \frac{\partial \Phi_2}{\partial x}\Big\vert_{x=l_{\mathrm{p}},-} = -\kappa_{\mathrm{eff,s}} \frac{\partial \Phi_2}{\partial x}\Big\vert_{x=l_{\mathrm{p}},+}$ & $-\kappa_{\mathrm{eff,s}} \frac{\partial \Phi_2}{\partial x}\Big\vert_{x=l_{\mathrm{p}}+l_s,-} = -\kappa_{\mathrm{eff,n}} \frac{\partial \Phi_2}{\partial x}\Big\vert_{x=l_{\mathrm{p}}+l_s,+}$
Negative electrode	7	$\varepsilon_{\mathrm{n}} \frac{\partial c}{\partial t} = D_{\mathrm{eff,n}} \frac{\partial^2 c}{\partial x^2} + a_{\mathrm{n}}(1-t_+) j_{\mathrm{n}}$ initial condition $c\big\vert_{t=0} = c_0$	$-D_{\mathrm{eff,s}} \frac{\partial c}{\partial x}\Big\vert_{x=l_{\mathrm{p}}+l_s,-} = -D_{\mathrm{eff,n}} \frac{\partial c}{\partial x}\Big\vert_{x=l_{\mathrm{p}}+l_s,+}$ & $-D_{\mathrm{eff,n}} \frac{\partial c}{\partial x}\Big\vert_{x=l_{\mathrm{p}}+l_{\mathrm{s}}+l_{\mathrm{n}}} = 0$
	8	$-\sigma_{\mathrm{eff,n}} \frac{\partial \Phi_1}{\partial x} - \kappa_{\mathrm{eff,n}} \frac{\partial \Phi_2}{\partial x} + \frac{2\kappa_{\mathrm{eff,n}} RT}{F}(1-t_+)\frac{\partial \ln c}{\partial x} = I$	$-\kappa_{\mathrm{eff,s}} \frac{\partial \Phi_2}{\partial x}\Big\vert_{x=l_{\mathrm{p}}+l_s,-} = -\kappa_{\mathrm{eff,n}} \frac{\partial \Phi_2}{\partial x}\Big\vert_{x=l_{\mathrm{p}}+l_s,+}$ & $\Phi_2\big\vert_{x=l_{\mathrm{p}}+l_{\mathrm{s}}+l_{\mathrm{n}}} = 0$
	9	$\sigma_{\mathrm{eff,n}} \frac{\partial^2 \Phi_1}{\partial x^2} = a_{\mathrm{n}} F j_{\mathrm{n}}$	$-\sigma_{\mathrm{eff,n}} \frac{\partial \Phi_1}{\partial x}\Big\vert_{x=l_{\mathrm{p}}+l_s} = 0$ & $\frac{\partial \Phi_1}{\partial x}\Big\vert_{x=l_{\mathrm{p}}+l_{\mathrm{s}}+l_{\mathrm{n}}} = -\frac{I}{\sigma_{\mathrm{eff,n}}}$
	10	$\frac{d}{dt} c_s^{ave} + 3\frac{j_n}{R_n} = 0$ *and* $\frac{D_{s,n}}{R_p}\left(c_s^{surf} - c_s^{ave}\right) = -\frac{j_n}{5}$	$c_s^{ave}\big\vert_{t=0} = c_{s,\max,n}$

Doyle-Newman RFM Equations*

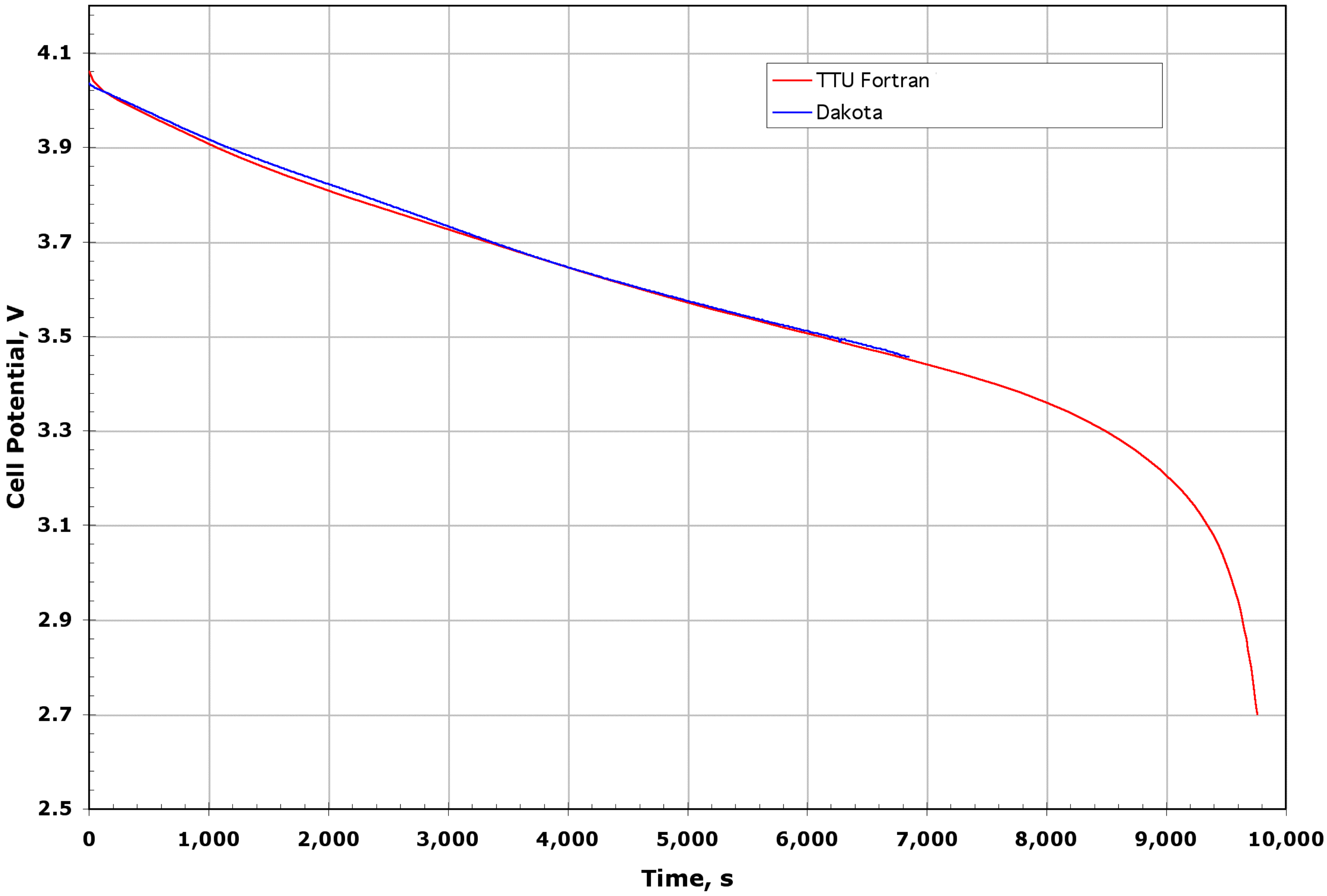
```
cg = YPRIME1 == -0.360988287612180473519614325667e0 * Y11 +
0.191473721423663165685371039105e1 * Y2 +
0.146117687123876805835205638937e1 * Y3 +
0.818581995016529393932356313404e0 * Y4 -
0.440732425220420596443425294418e-1 * Y12 -
0.719697867284305954134430075150e-2 * Y13 -
0.685083539666203007516357670348e-4 * Y27 +
0.978449599957300704744211515242e-3 * Y17 +
0.276798199212208598538807863935e-2 * Y16 +
0.581291671447654875471851298803e-2 * Y15 -
0.112100335291330779227032034152e-2 * Y26;

cg0 = YPRIME2 == -0.104734249360964342981939099480e3 * Y11 +
0.104656672129568664601261175017e4 * Y2 +
0.103798289326955751327984326349e4 * Y3 +
0.718675841738942734239822899829e3 * Y4 -
0.502628862439300239490175953060e2 * Y12 -
0.188673916717988074563774446292e2 * Y13 +
0.893992957759775113797091423114e2 * Y15 +
0.373979432853879040408243999827e1 * Y27 -
0.127185420572778699829649815127e2 * Y17 -
0.410247122066572230038398906012e2 * Y16 -
0.701132161249252879771610214910e1 * Y26;
```

* - *Two of the shortest equations shown for illustration*

Doyle-Newman Chemistry



TTU / USG Chemistry



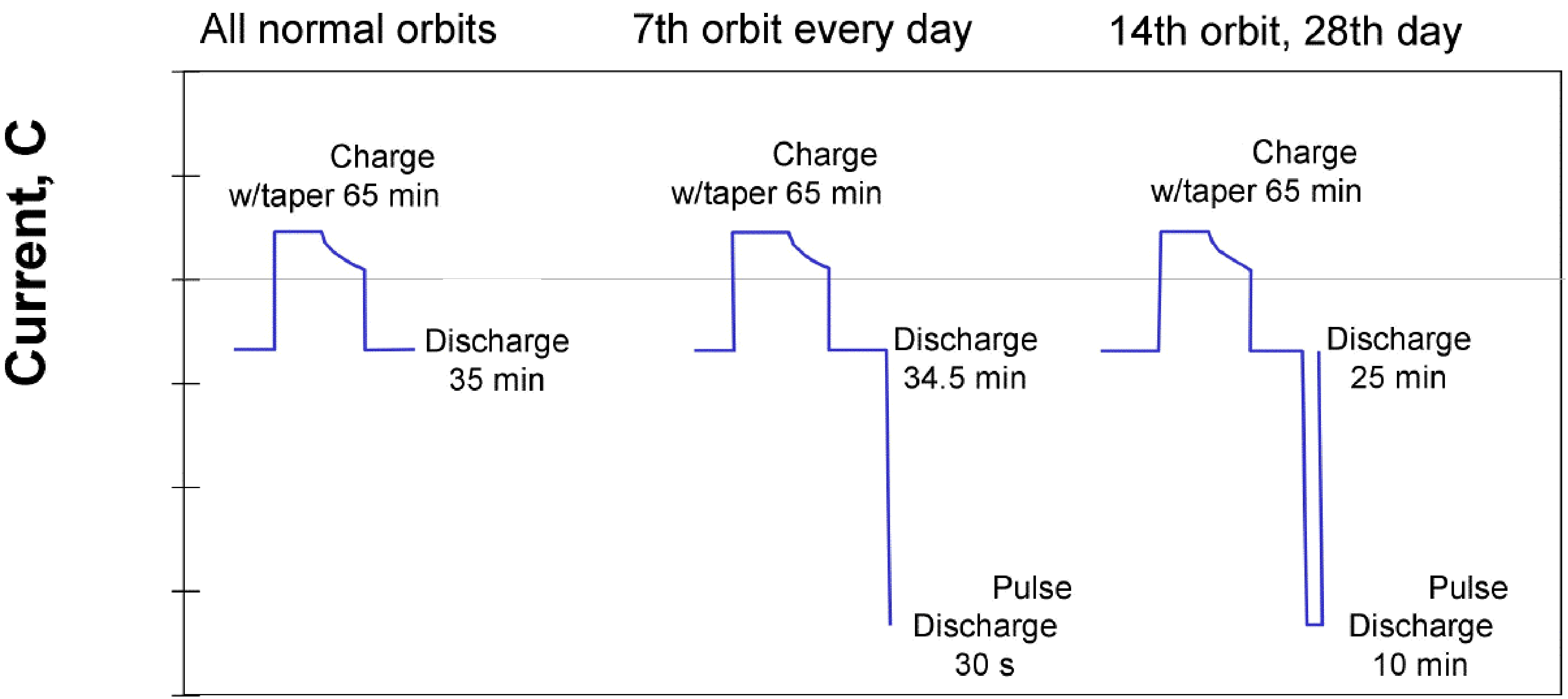
Proof-of-Concept RFM Equations

- Doyle-Newman Cell Model ($LiMn_2O_4$)
- 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

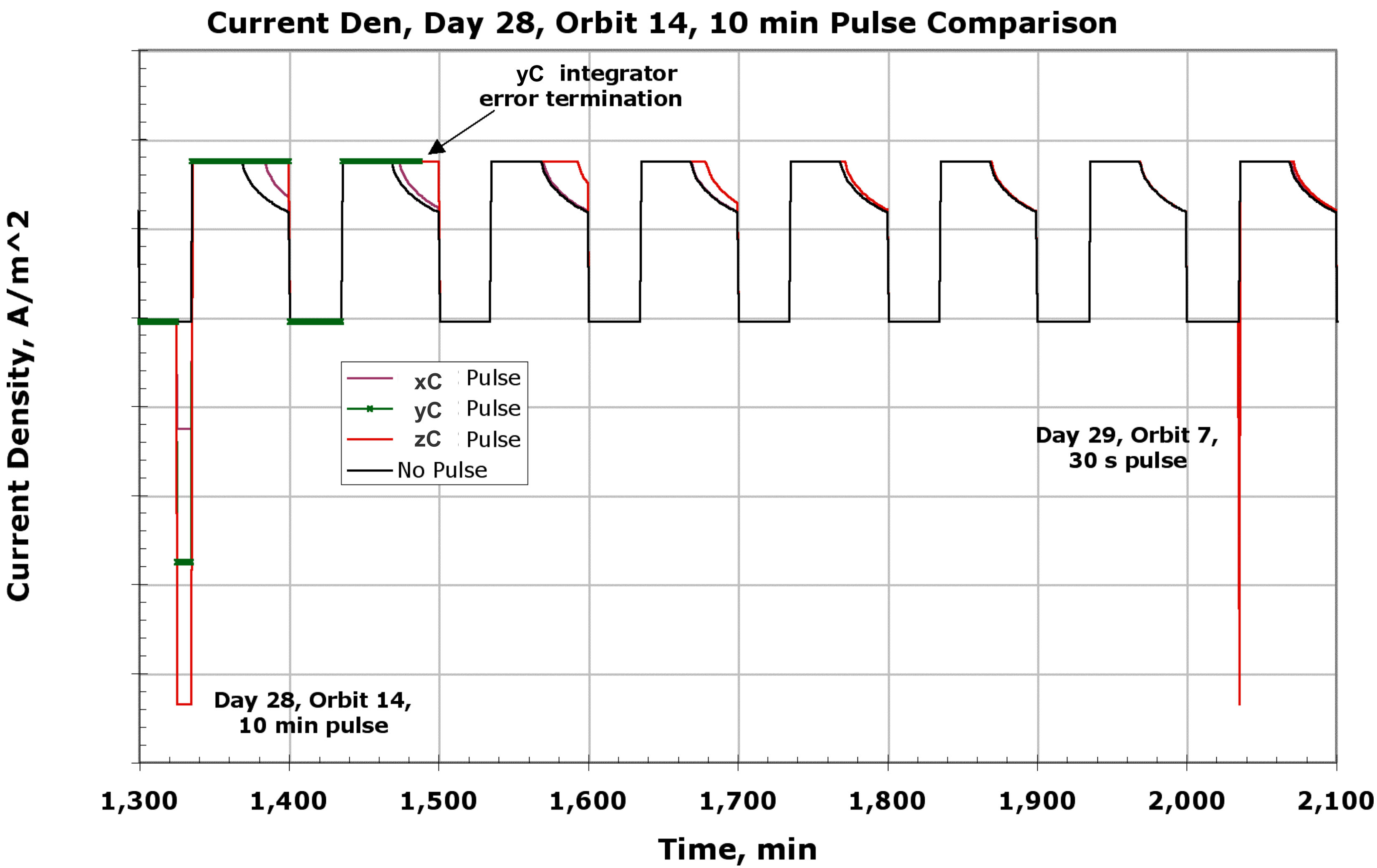
Example Cycling Regime Assumptions

- 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

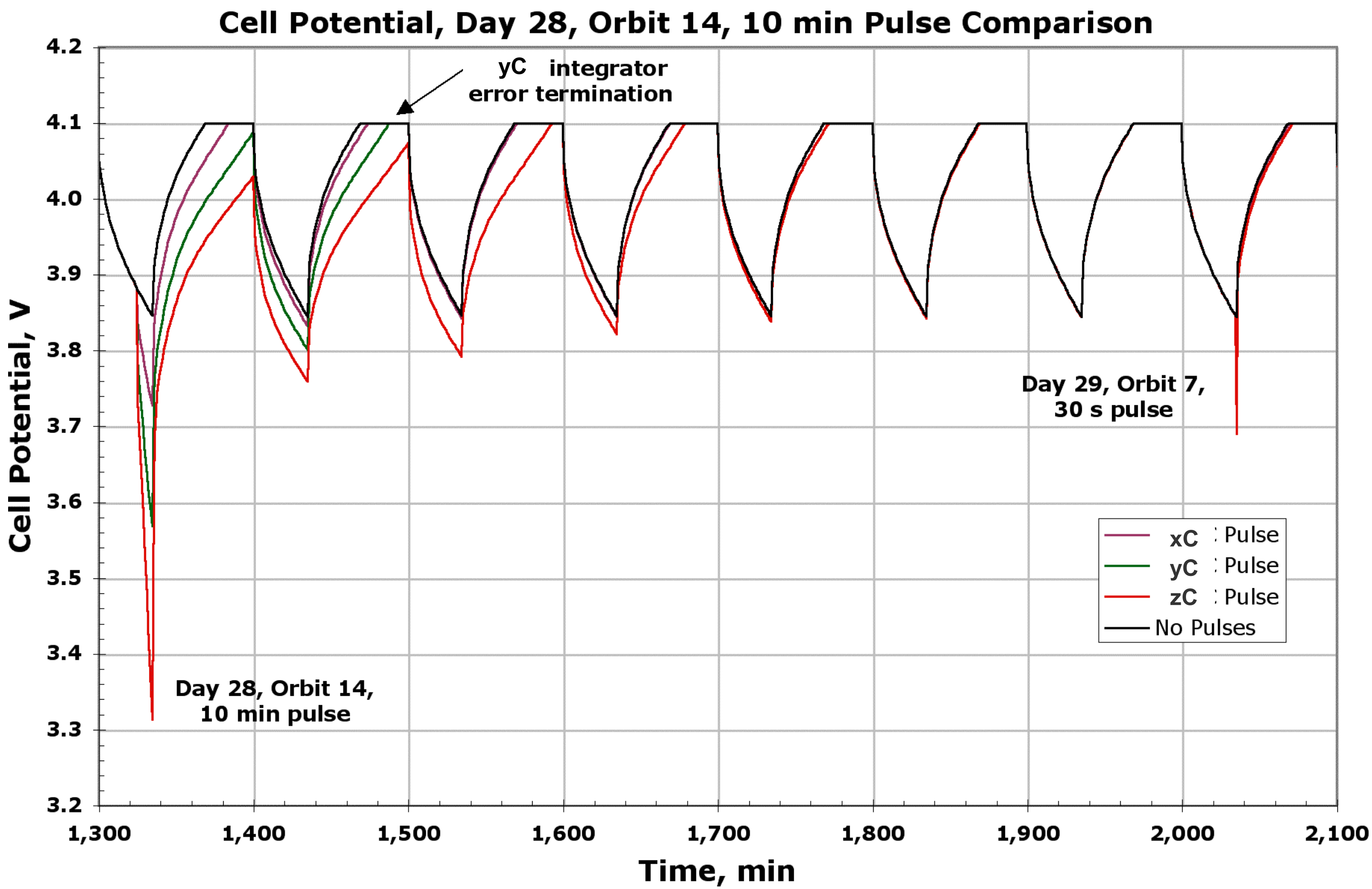
Cycling Regime Schematic



Pulse and No-pulse Comparison: Current Density



Pulse and No-pulse Comparison: Cell Potential



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

Global Aerospace Corporation is appreciative of the support of MDA and specifically

Dr. Harlan Lewis for his direction