



Development of Computer-Aided Design Tools for Automotive Batteries



Steve Hartridge, CD-adapco
June 17th 2014

Project ID:
ES118

Overview



Timeline

- Started – August 1st 2011
- Finished – July 31st 2014
- Currently – 90% completed

Barriers Addressed

- Excessive time & cost for cell & pack design process
- Lack of design exploration
- Limited existing methods for analysis

Budget

- Total project funding \$2.74M (3 Years)
 - \$1,370,313 DoE
 - \$1,370,313 CD-adapco team (50%)

Partners

- Battery Design LLC
 - Johnson Controls
 - A123 Systems Inc
 - NREL
 - ORNL
- + Idaho National Labs
- Electrolyte information

Funding provided by Dave Howell of the DOE Vehicle Technologies Program .
The activity is managed by Brian Cunningham of Vehicle Technologies.
Subcontracted by NREL, Kandler Smith Technical Monitor

Objectives/Relevance



Supporting DoE's Vehicle Technology Programs Targets

- Reducing PHEV & EV battery costs through the application of simulation and computer aided design

Supporting DoE's CAEBAT Objectives

- Significant reduction in design cycles and optimization of batteries
- Address the barriers of cost, performance, life and safety with quantitative tools

Project Objectives

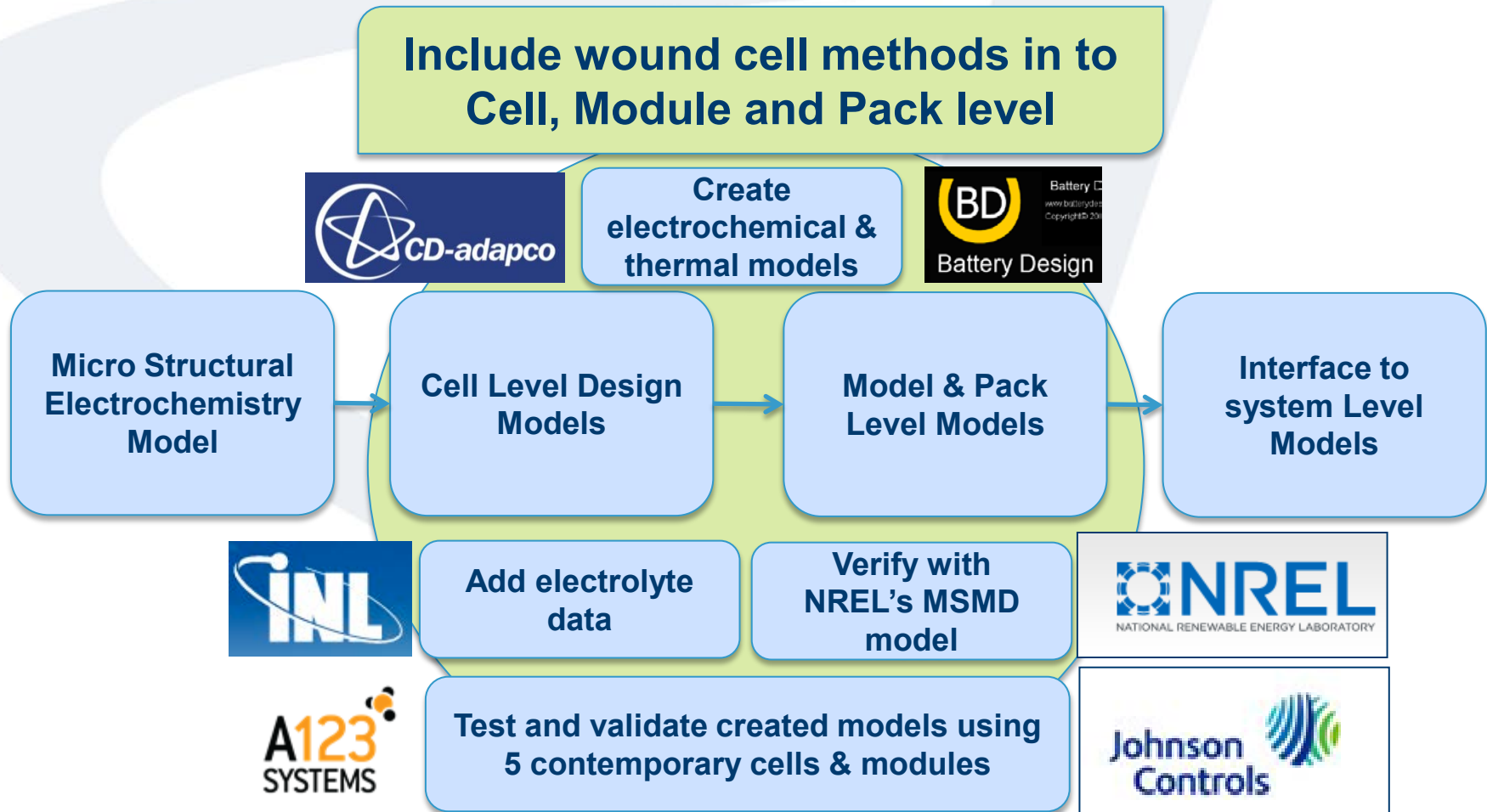
- To produce electrochemical, electrical, and thermal simulation models applicable for spirally wound lithium ion cell designs, both cylindrical and prismatic
- Validate the results of the simulation across a range of lithium ion cell chemistries
- Generate best practice methods for the timely generation of future electrochemical models by users
- Include the created simulation models and best practice into the readily available 3D multi-physics code STAR-CCM+, for combined flow, thermal & electrochemical simulation across a range of length scales.

Milestones Status



Month/Year	Milestone	Status
June 2013	Detailed Electrolyte database included	Done
June 2013	Calendar ageing model available	Done
September 2013	VL6P cell model, single cell model & 12 cell module simulations completed	Done
October 2013	Release of simulation Code to Project	Done
December 2013	Completion of all 4 module tests at JCI	Done
March 2014	Released of simulation code in CD-adapco's STAR-CCM+ code, used by project partners	Done
April 2014	Completion of all 5 module simulations and method validation	Done
May 2014	Code to code verification with NREL's MSMD paper	On track
May 2014	ORNL validation of open architecture compatibility	On track
June 2014	Final report and results	On track

Project Strategy



- CD-adapco is coordinating the project
- Develop method to characterize cell information from controlled cell tests to create a robust simulation model
- Produce validation simulations for a range of wound cell types
- Expand limits of the electrochemistry model to increasingly abusive conditions

Technical Approach



- An industrially relevant, easy to use, electrochemical and thermal model has been created which can be applied to wound electrode battery types. This model is applicable at both the cell and module and pack level of analysis, the fidelity of the model can be controlled by the users depending on their desired output and level of accuracy
- 5 cells from 2 different manufacturers and spanning the 3 cell form factors (stacked, cylindrical and prismatic wound electrodes) have been used to validate the computational model developed using real world drive cycles. This also included a “blind” validation using a WLTC drive cycle on one module
- A database has been added which features 12 contemporary electrolyte formulations, typical of those used in modern lithium ion batteries. This enables the a more complete physics based simulation to take place
- A process to generate the electrochemical model using cell information and controlled test work has been validated within the project
- A complimentary calendar aging model has been created which works alongside the created cell performance models preconditioning them to an “aged” stage
- The approach has been extended in to the system level space using either an electrochemical approach or reduced order models

Publications

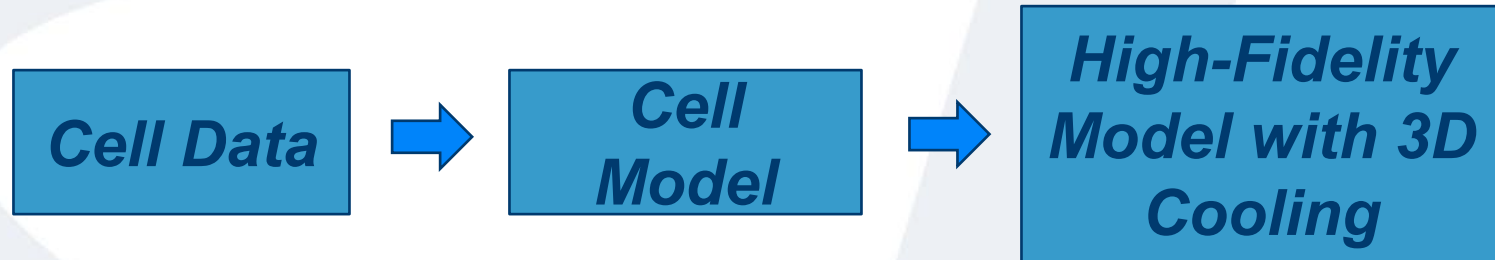
Design and Simulation of Spirally-Wound, Lithium-Ion Cells Lithium-Ion Batteries: Modeling

R. Spotnitz, S. Hartridge, G. Damblanc, G. Yeduvaka, D. Schad, V. Gudimetla, J. Votteler, G. Poole, C. Lueth, C. Walchshofer, and E. Oxenham, ECS Transactions 2013 50(26): 209-218.

Simulation of Electrolyte Composition Effects on High Energy Lithium-Ion Cells

R. Spotnitz, K. Gering, S. Hartridge, G. Damblanc, ECS Transactions 2014, to be published.

Technical Approach



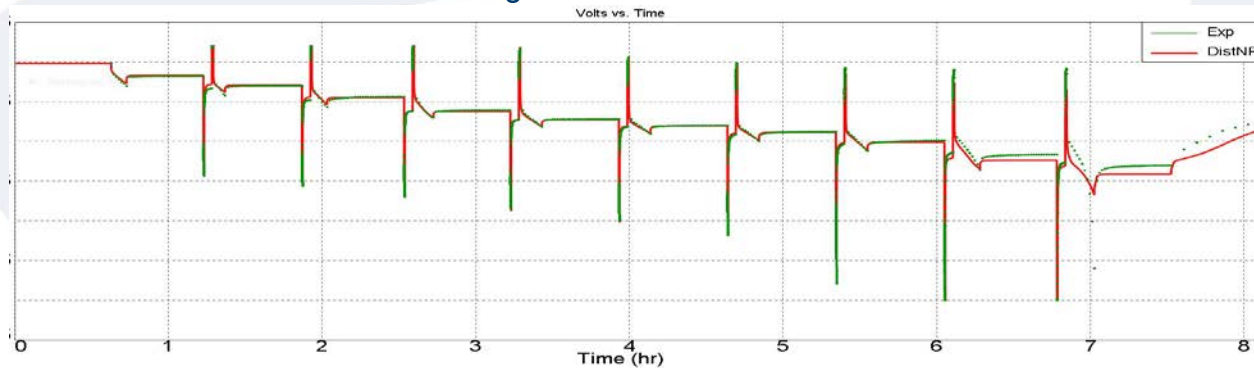
- **Cell Characterization Data**
 - HPPC, CC tests done at several temperatures
 - Temperature should be well-controlled. This improves temperature-dependence of modeling parameters. Parameter fitting is done with low-order cell & thermal model.
- **Cell Model**
 - Cell parameters iteratively fitted
 - Model runs quickly due to low electrical & thermal resolution
 - Complete model definition contained in single file
- **3D High definition Model**
 - Higher (variable) electrical resolution
 - 3D thermal model based on CAD data. Allows complex thermal effects such as radiation, convection, contact resistances.

Technical Approach

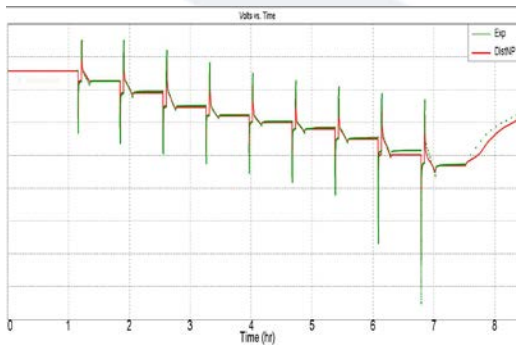


- Cell Model vs Characterization Test

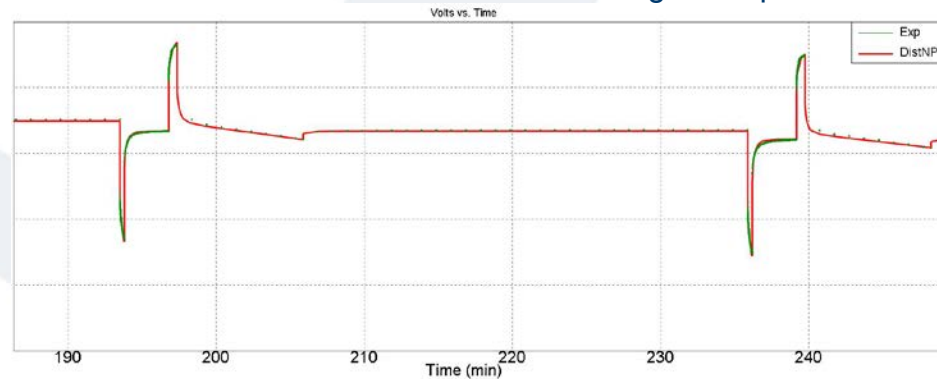
20 C Rate HPPC at 35 deg



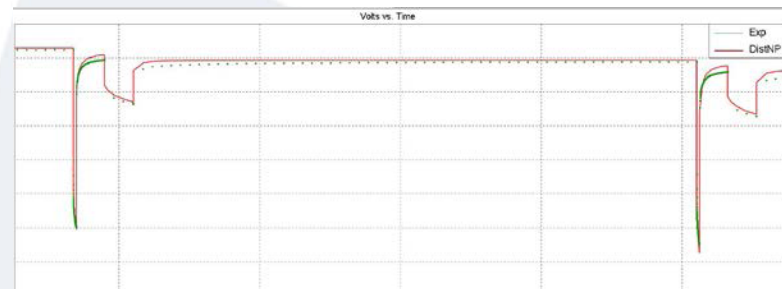
20 C Rate HPPC at 10 deg



20 C Rate HPPC at 10 deg – two pulses



10C Rate HPPC at -10 deg



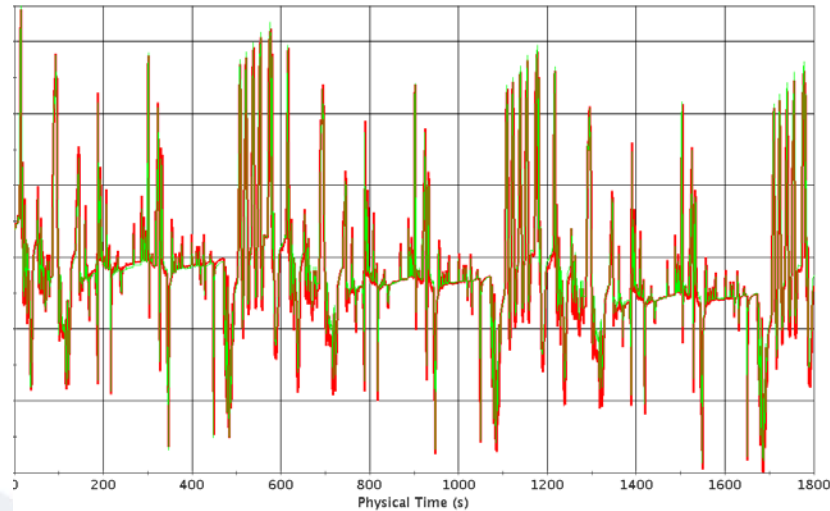
Technical Approach



- 3D Cell Model vs Drive Cycle Test

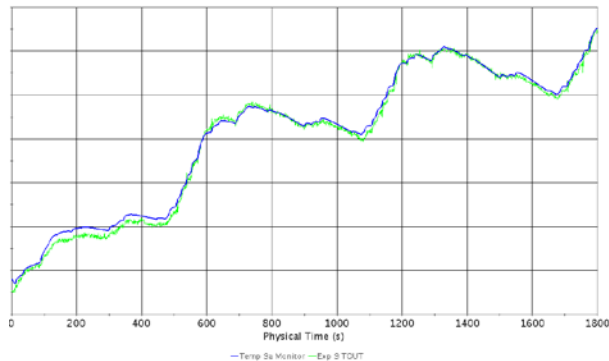
Cell Voltage

Voltage Cell 09 Monitor Plot



Example Thermocouple positions

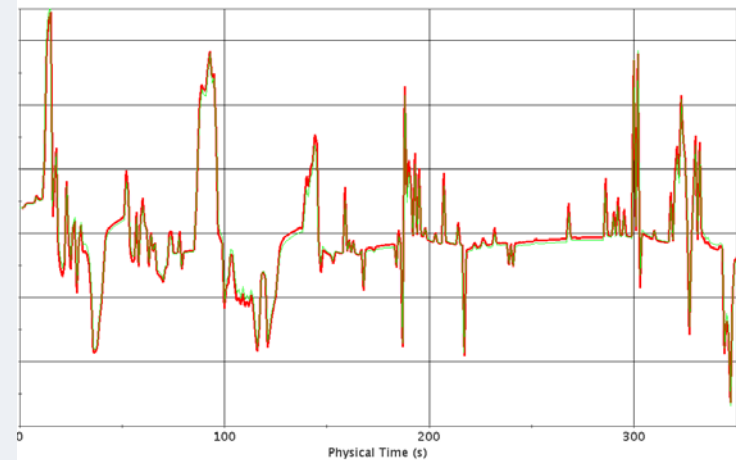
Cell 9a Temperatures



Cell Temperature - Top

Cell Voltage – First 300 Seconds

Voltage Cell 09 Monitor Plot



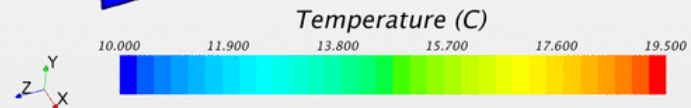
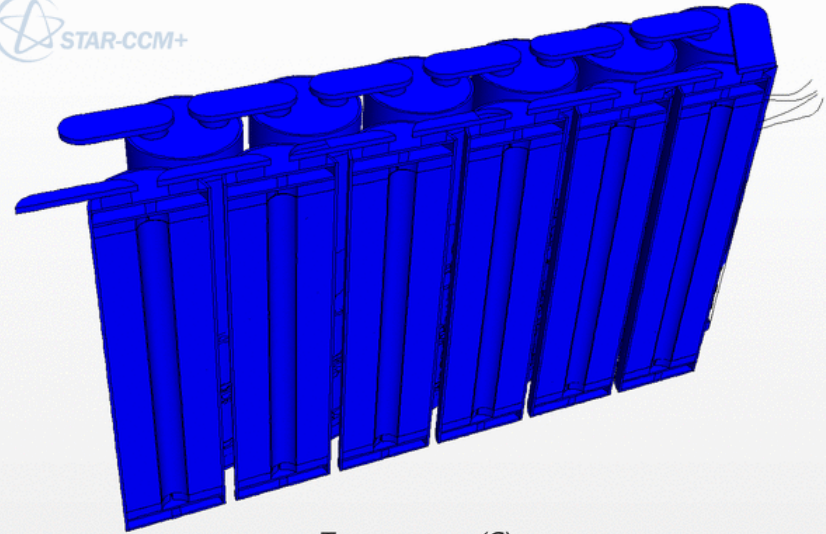
Technical Approach



- 3D Module Model vs Drive Cycle Test

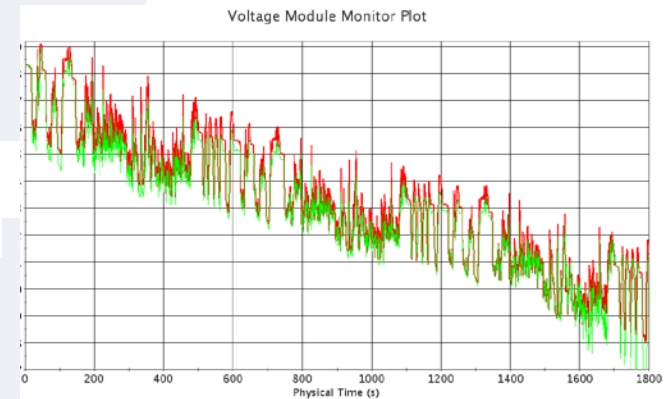


VL6P 12-Cell US06 Drive Cycle



Solution Time 10 (s)

Cell Voltage

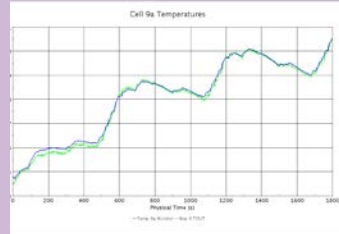
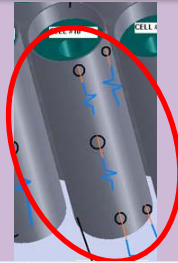
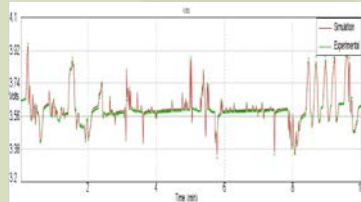
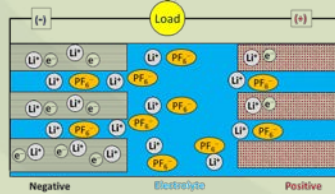


Application of Approach

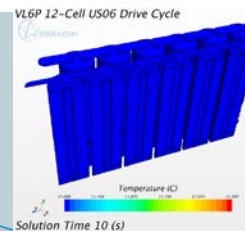


Example Results

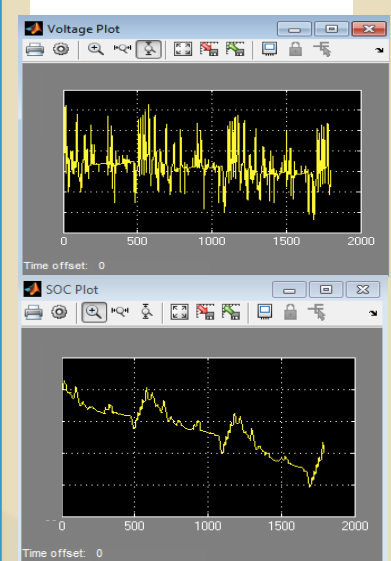
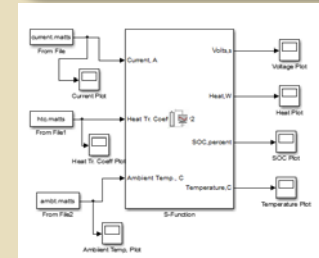
**Cell Level Design Models
(lumped or 3D models)**



**Model & Pack
Level Models
(3D models)**



**System Level
Models
(lumped)**



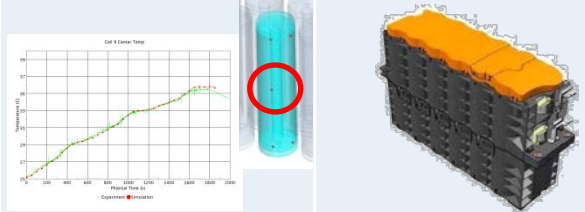
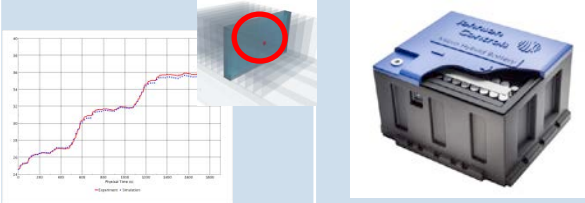
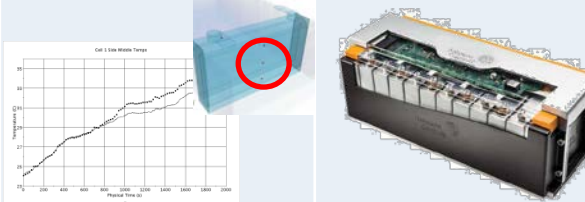
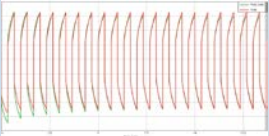
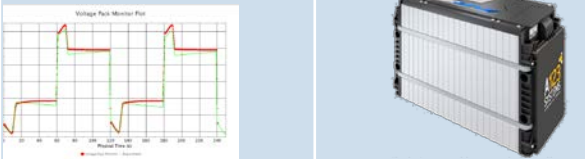
**Model
Type**

**Electrical
Results**

**Thermal
Results**

Application of Approach

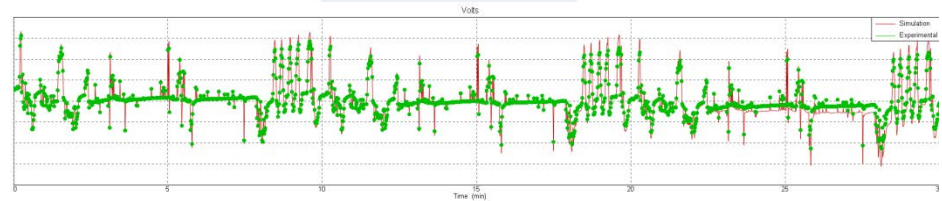


Cell Description	Cell Type	Model used	Cell Results for US06	Module results	
VL6P 	Wound cylindrical	Electrochemical + wound cell method	9.2mv (rms)		
VL41M 	Wound cylindrical	Electrochemical + wound cell method	13.2mv (rms)		
PL6P 	Wound prismatic	Electrochemical + wound cell method	12.1mv (rms)		
PL27M 	Wound prismatic	Electrochemical + wound cell method	6.5mv (rms)		
A123 20Ahr 	Stack	Reduced order equivalent circuit + pouch method			

Extensions to Approach

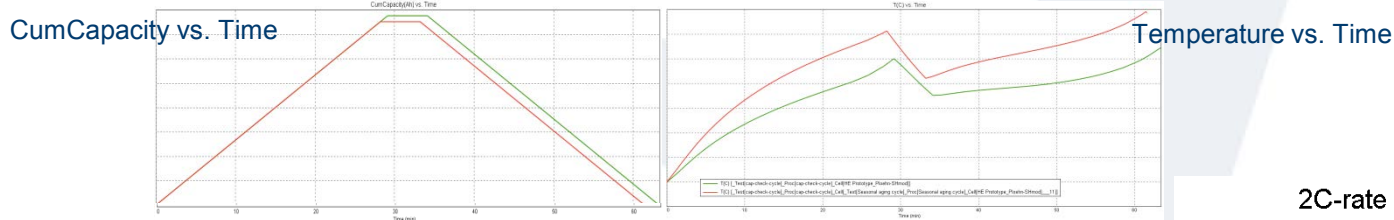
- **Reduced Order Models for System Simulations**

- Equivalent circuit model generated from synthetic data produced by electrochemistry model
- RMS error compared (21mV vs. 9mV)
- Runtime compared (6 seconds for reduced order model vs 11 minutes for echem model)



- **Calendar Ageing Model**

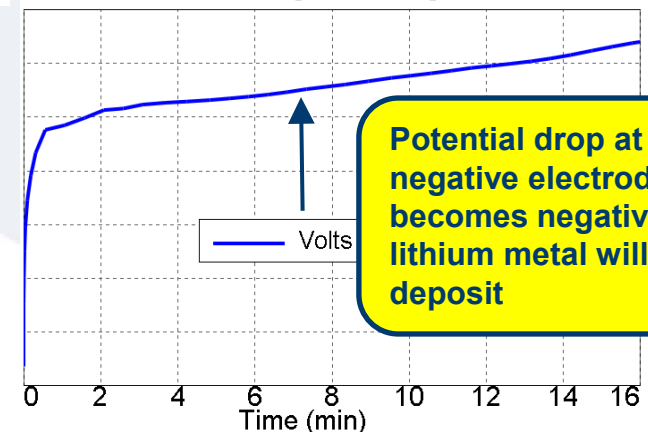
- Based on the work of Pleohn et al.
- Can be used to pre-condition a cell to a given aged state before running a simulation



- **Low Temperature Charge Simulation**

- Using electrochemical model
- Highlight when the negative electrode potential goes below 0V for given charge/temperature conditions
- Follows USABC procedure

2C-rate charge at -10degC



Verification of Approach



- Comparison to NREL's Multi Scale Multi Dimension paper using the newly created approach and tools.

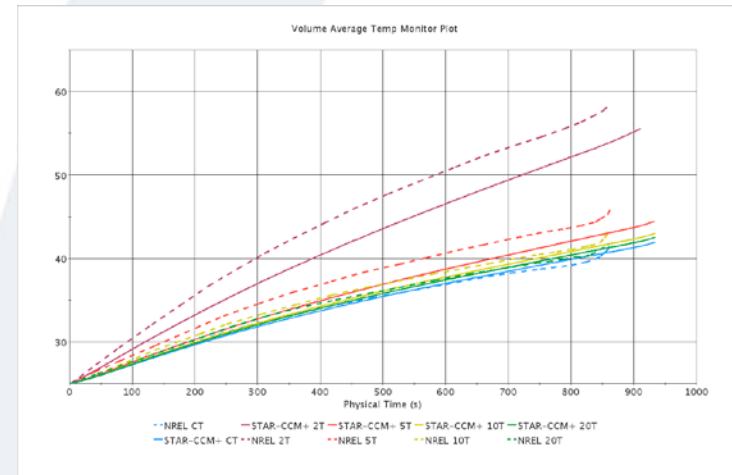
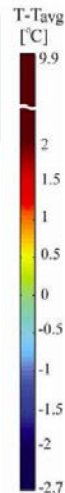
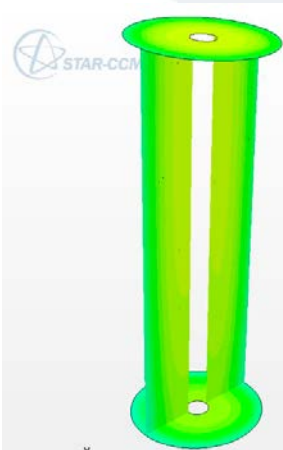
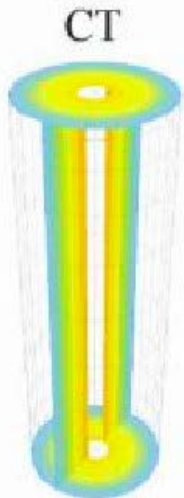


Journal of The Electrochemical Society, **158** (8) A955-A969 (2011)
0013-4651/2011/158(8)/A955/15/\$28.00 © The Electrochemical Society

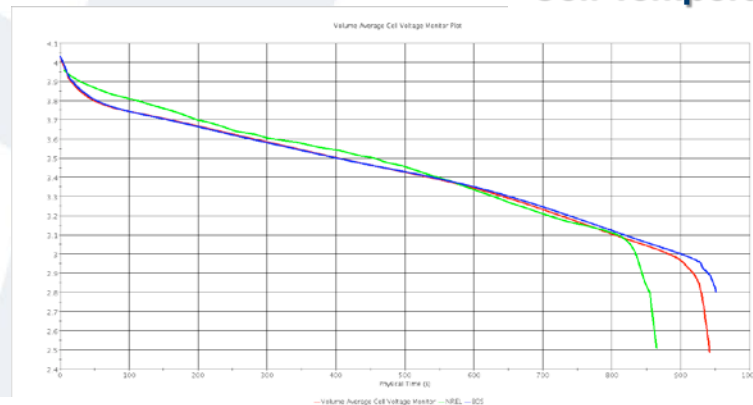
Multi-Domain Modeling of Lithium-Ion Batteries Encompassing Multi-Physics in Varied Length Scales

Gi-Heon Kim,^{*,*} Kandler Smith,^{*} Kyu-Jin Lee,^{*} Shriram Santhanagopalan,^{*} and Ahmad Pesaran

National Renewable Energy Laboratory, Golden, Colorado 80401, USA



Cell Temperature



Cell Voltage

Collaborations



- The major collaboration is between CD-adapco and Battery Design LLC to create the framework and also JCI to understand the details of testwork and complete the validation.
- The project is collaborating with NREL's energy storage team on code to code verification of the models behavior for defined cells, this compares results to NREL's in-house MSMD code
- The project is collaborating with NREL and Oak Ridge National Lab on creating an open architecture software framework to allow model transfer between CAEBAT projects
- The project has also worked with Dr K. Gering at Idaho National Lab for the inclusion of the detailed electrolyte data in to the modeling framework

Publications and Presentations



Design and Simulation of Spirally-Wound, Lithium-Ion Cells Lithium-Ion Batteries: Modeling

R. Spotnitz, S. Hartridge, G. Damblanc, G. Yeduvaka, D. Schad, V. Gudimetla, J. Votteler, G. Poole, C. Lueth, C. Walchshofer, and E. Oxenham, ECS Transactions 2013 50(26): 209-218.

Simulation of Electrolyte Composition Effects on High Energy Lithium-Ion Cells

R. Spotnitz, K. Gering, S. Hartridge, G. Damblanc, ECS Transactions 2014, to be published.

Thermal & Electrochemical Simulation of Automotive Battery Pack Systems

S. Hartridge, G. Damblanc, R. Spotnitz, presented at the Automotive Advanced Batteries Conference, Atlanta, 7th February, 2014

Responses to Reviewer Comments



“Any significant focus on standardized battery CAE software did not support overall DOE objectives as monopolization of this industry could stifle both innovation and further advancement”

The CAEBAT program is a competitive process and funded 3 vendors in the same field. Any consensus should be focused on the equation sets to be solved not tools to be used, this will be decided by the market

“collaboration with JCS and A123 was good, but additional collaboration with other, more diverse battery developers would be even better.”

The presented methods are now in CD-adapco’s released code and being used by a wide users base in the US, Europe, Japan, Korea & China.

“This reviewer felt uncertain of the background on potential particular focus on electrolyte properties for future work. The same reviewer inquired about binder properties, separator properties, etc.”

By including the electrolyte data the fits to test work were improved. Moreover having such a database improves the usability of the overall methods.

Summary



This project has delivered an integrated multi length scale approach to battery analysis within computer-aided engineering. This is delivered within the wide spread CAE tool STAR-CCM+

The latest version of STAR-CCM+ with the CAEBAT developed models was released to public in February 2014

The approach has been validated on a number of commercial lithium ion cells/modules which have been reported in this and other presentations

Thanks to DOE's CAEBAT program, these methods are in use within the US and other global locations with a growing commercial user base and making a positive impact on the design of future HEV's & EV's battery systems.