Energy Storage R&D
Thermal Management Studies and Modeling

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ES_12_Pesaran

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This presentation does not contain any proprietary or confidential information.

NREL Energy Storage Program

Our projects support the three major elements of DOE's integrated Energy Storage Program to develop advanced energy storage systems for vehicle applications.

- Battery Development, Testing, Analysis
  - Thermal characterization and analysis
  - Energy storage simulation and analysis
- Applied Battery Research
  - Li-ion thermal abuse reaction modeling

Will be discussed in this presentation.

- Exploratory Battery Research
  - Nano-structured metal oxide anodes

Will be discussed by Anne Dillon on Thursday morning.

Outline

Discussion of ***three*** *activities funded*

We will discuss most of these for each section:

- Objective
- Barriers
- Approach
- Accomplishments
- Future Work/Plans
- Summary
- Response to comments
- Publications

1. Thermal Characterization and Analysis
2. Energy Storage Simulation and Analysis
3. Li-ion Thermal Abuse Reaction Modeling

Overview

Timeline

- Project start date: Oct 2004
- Project end date: Sep 2013
- Percent complete: 60%

Partners

- USABC
- A123 Systems
- CPI/LG Chem
- EnerDel
- Johnson Control Saft
- General Motors
- General Atomics
- NASA

Barriers

- Decreased life at high temperatures (15 years target)
- Safety concerns due to thermal runaway
- High cost due to high cells cost and system integration

Budget

- Funding received in
  - FY08: $1.20M
  - FY09: $1.40M

Objectives/Milestone/Approach

- **Objectives** (Task 6 of the DOE's Vehicle Technologies R&D Plan)
  - Measure thermal properties of batteries and ultracapacitors
  - Model thermal performance of batteries
  - Support USABC and FreedomCAR developers
- **Milestones**
  - Thermal evaluation of advanced batteries (August 2008 and June 2009)
  - Electro-chemical-thermal based battery models (July 2008 and August 2009)
- **Approach**
  - **Work with developers** on thermal characterization, evaluation, and modeling of cells, modules, and packs
  - Use NREL's collective experimental and modeling capabilities to support developers in addressing issues of battery thermal management and performance

Thermal Characterization Approach

Cells, Modules and Packs

Tools:
- Calorimeters
- Thermal imaging
- Electrical cyclers
- Environmental chambers
- Dynamometer
- Vehicle simulation tools
- Thermal analysis tools

Test Profiles:
- Normal operation
- Aggressive operation
- Driving cycles
  - US06
  - UDDS
  - HWY
- Discharge/charge rates
  - Constant current
  - Geometric charge/discharge cycles
  - FreedomCAR profiles

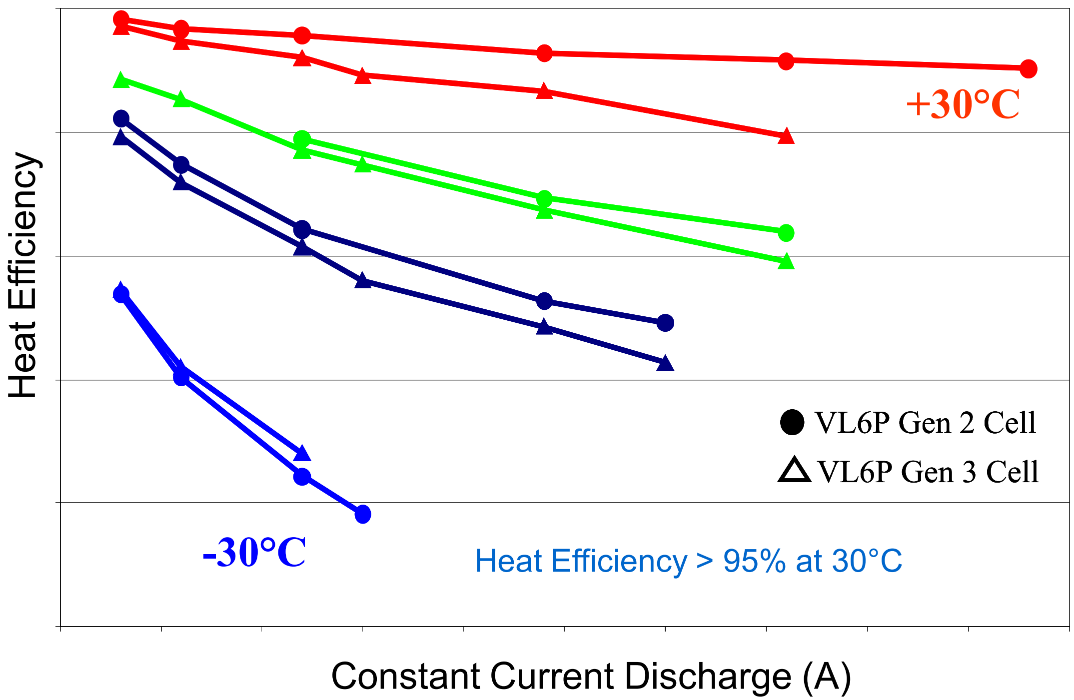
Measurements:
- Heat capacity
- Heat generation
- Efficiency
- Thermal performance
  - Spatial temperature distribution
  - Cell-to-cell temp. imbalance
  - Cooling system effectiveness

Results reported to DOE, USABC, and developers

Thermal Characterization: Johnson Controls- Saft Low-Temp. HEV Cells

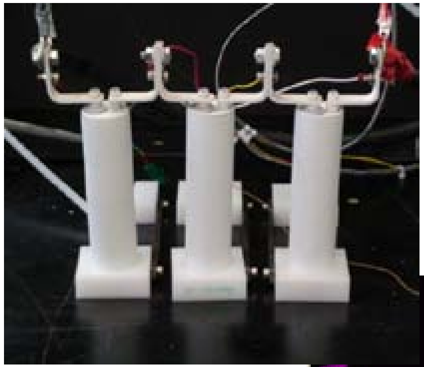
Calorimetry

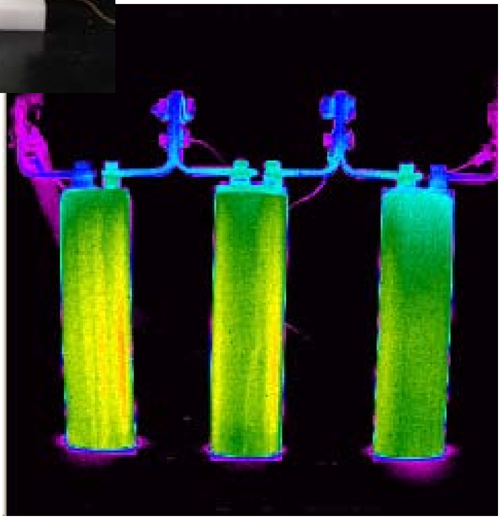
- Heat capacity & heat generation & **efficiency**
- Temperatures: -30 to +30˚C
- Profiles: USABC 25 & 50 Wh cycles, CC discharge



Thermal Imaging at 12C Rate

- Temperatures: Ambient
- Profiles: 100% SOC to 0% SOC

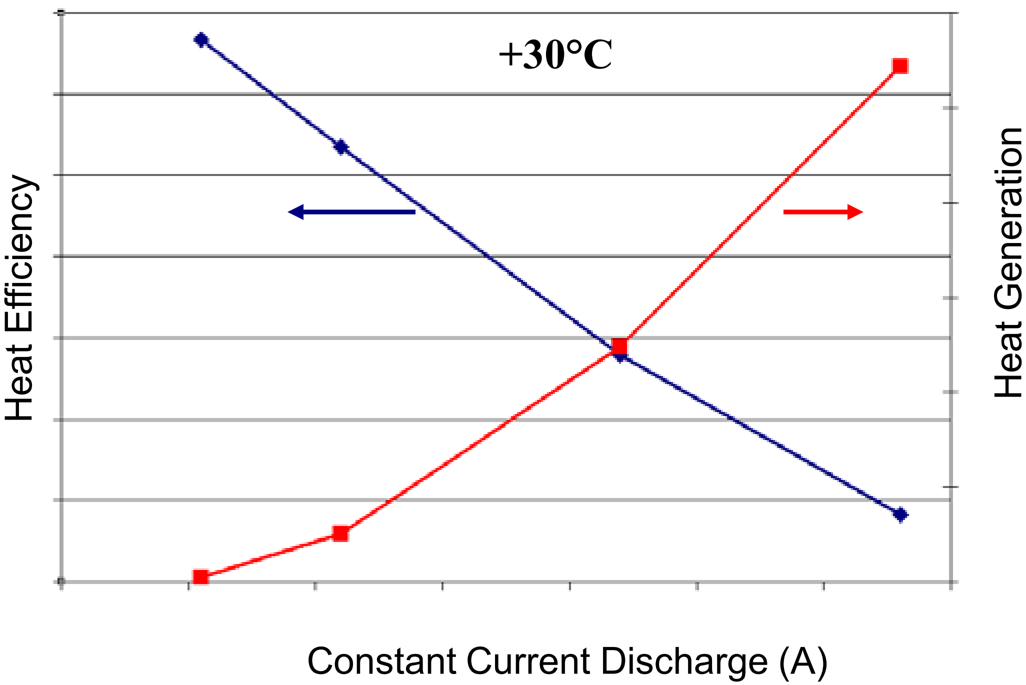




Thermal Characterization: Johnson Controls- Saft PHEV VL22M Cells

Calorimetry_

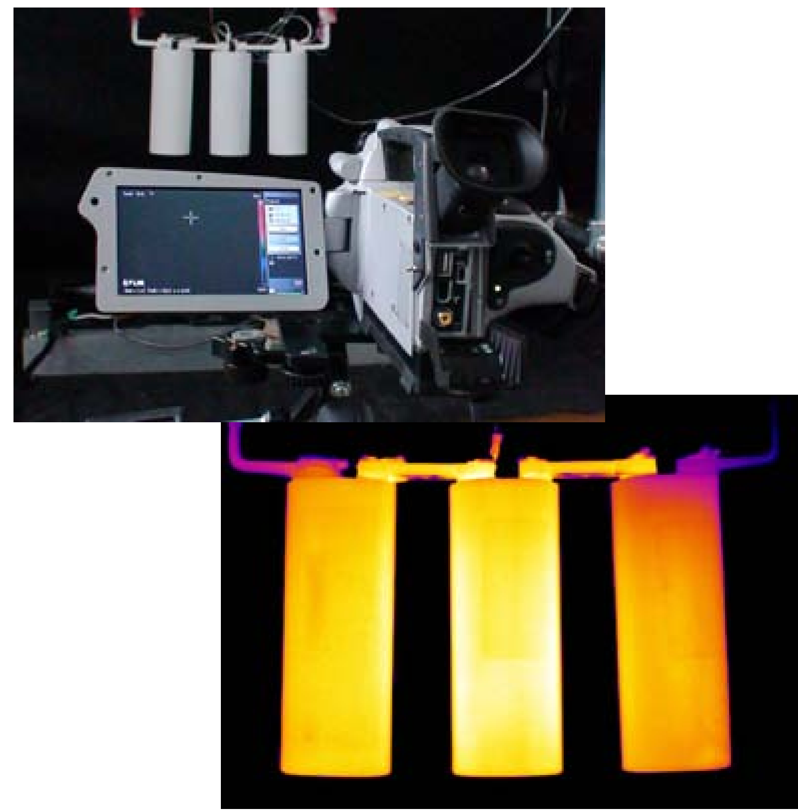
- Heat capacity & heat generation & **efficiency**
- Temperatures: -30 to +30˚C
- Profiles: CC discharge



Heat Efficiency > 90% for currents < 5C rate at 30°C

Thermal Imaging

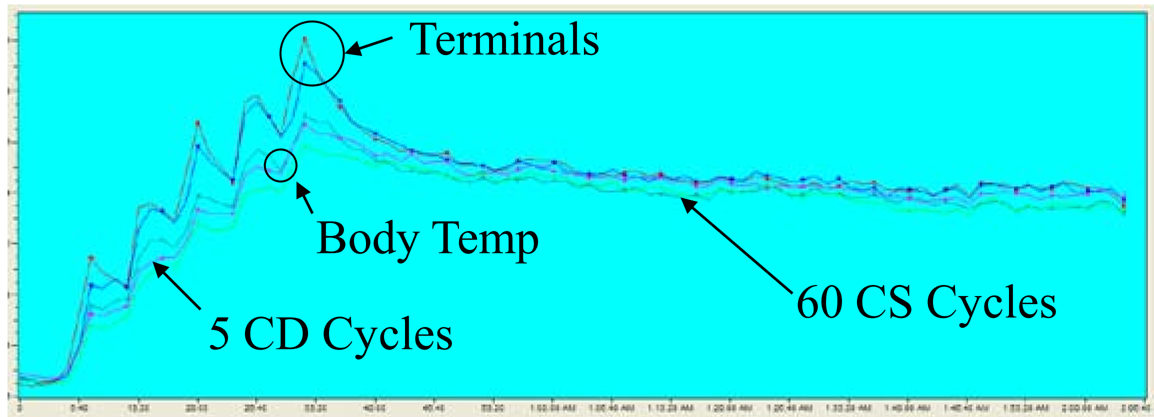
- Temperatures: Ambient
- Profiles: 100 Amp Geometric Cycle, 5C Discharge



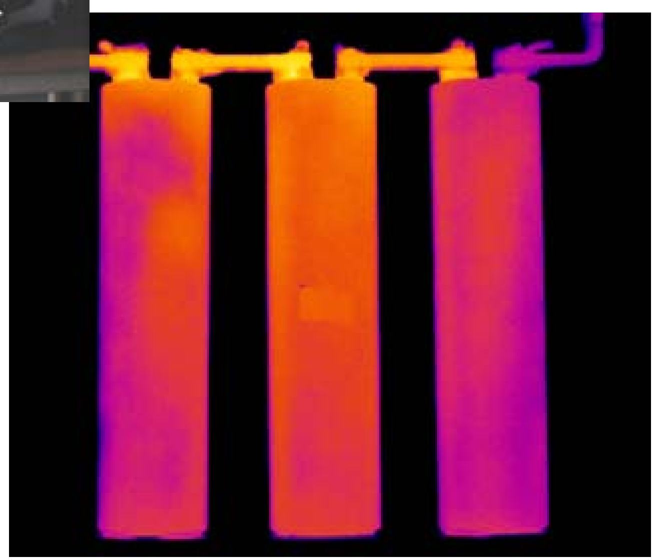
Thermal Characterization: Johnson Controls-Saft PHEV VL41M Cells

Thermal Imaging

- Temperatures: Ambient
- Profiles: CD PHEV Cycle, CS PHEV Cycle, Geometric Cycles, CC Discharge



Center Cell Temp Profile



CD: Charge Depleting
CS: Charge Sustaining

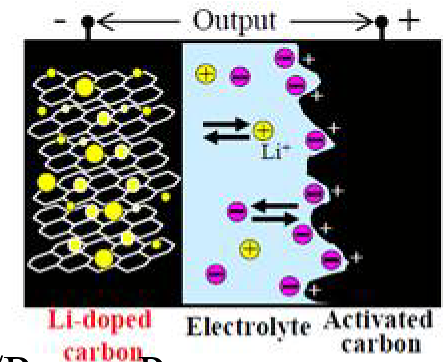
Calorimetry Future Work

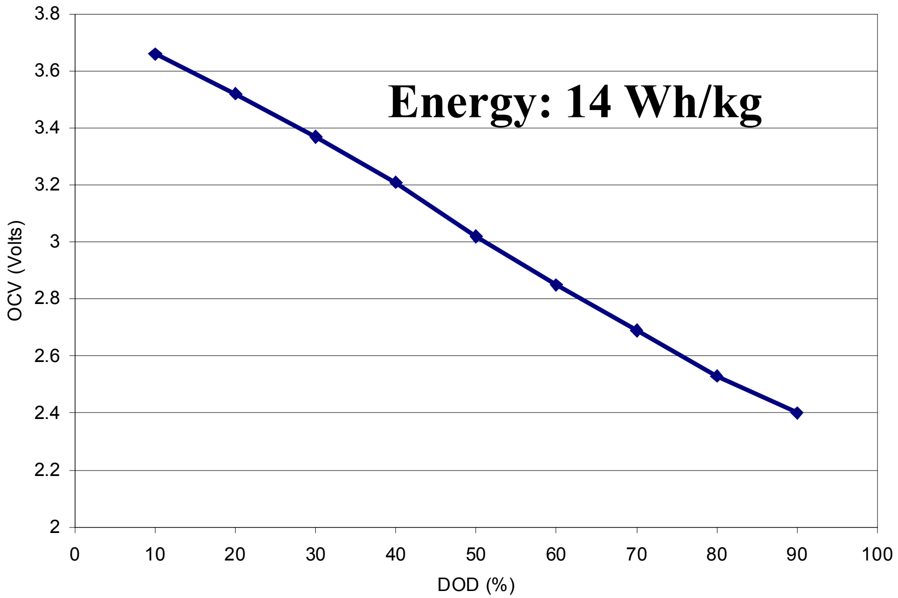
- Heat capacity & heat generation & **efficiency**
- Temperatures: -30 to +30˚C
- Profiles: CC discharge, CD PHEV, & CS PHEV

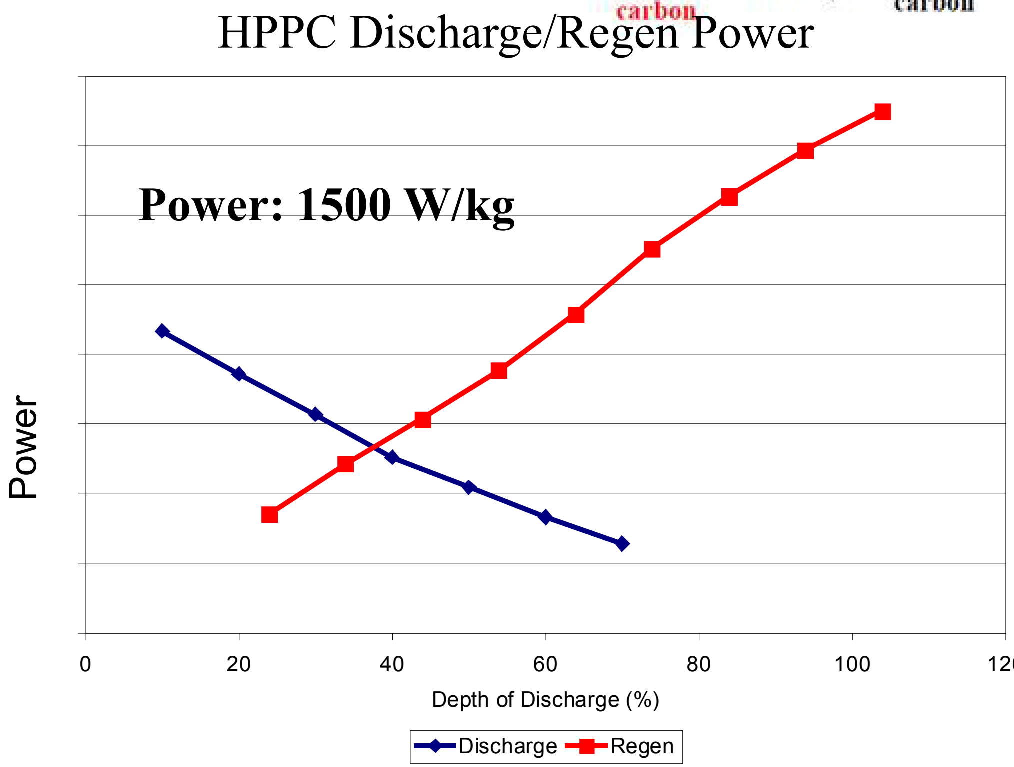
JSR Micro MATERIALS INNOVATION JSR

Electrical Characterization: Lithium Ion Capacitor Cells

- C/1, 10C, 100C, and HPPC Testing







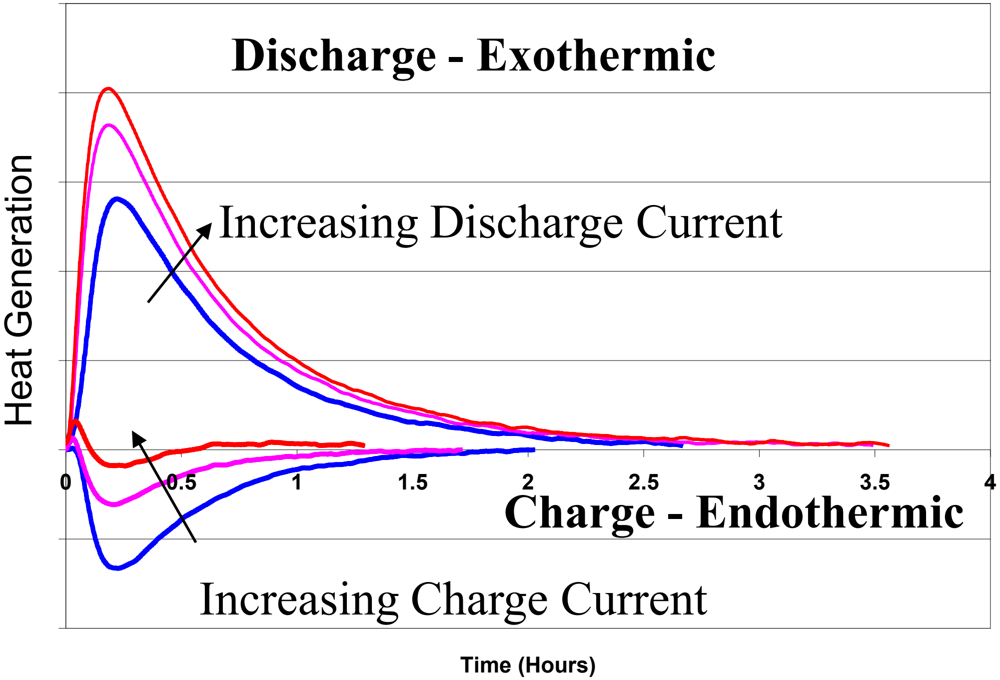
This asymmetric capacitor had high resistance; the next generation is claimed to be better.

JSR Micro MATERIALS INNOVATION

Thermal Characterization: Lithium Ion Capacitor 2200 F Cells

Calorimetry_

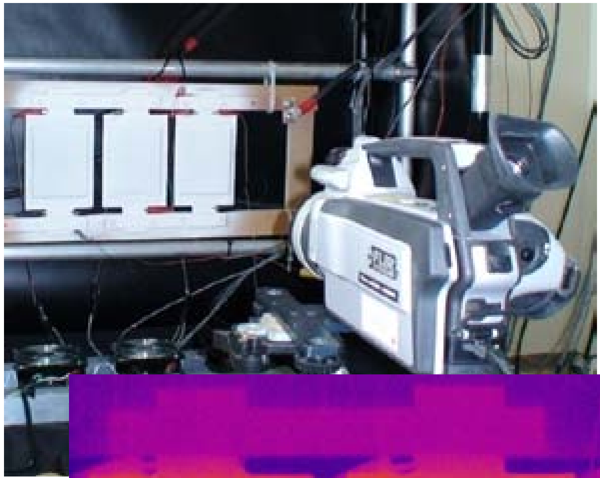
- Heat capacity & heat generation & **efficiency**
- Temperatures: +30˚C
- Profiles: CC discharge cycles

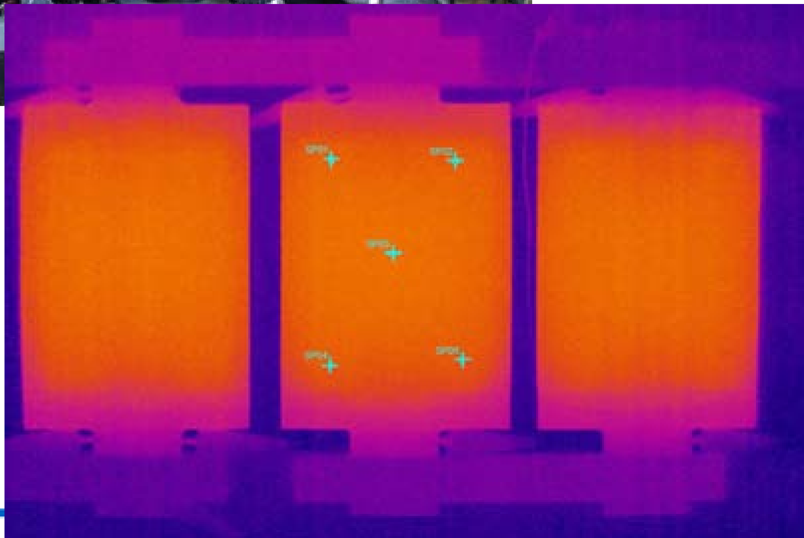


Calorimeter Response to Constant Current Charge/Discharge

Thermal Imaging

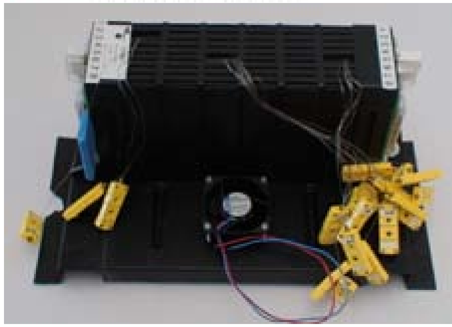
- Temperatures: Ambient
- Profiles: 50C, 100C, and Geometric Cycle

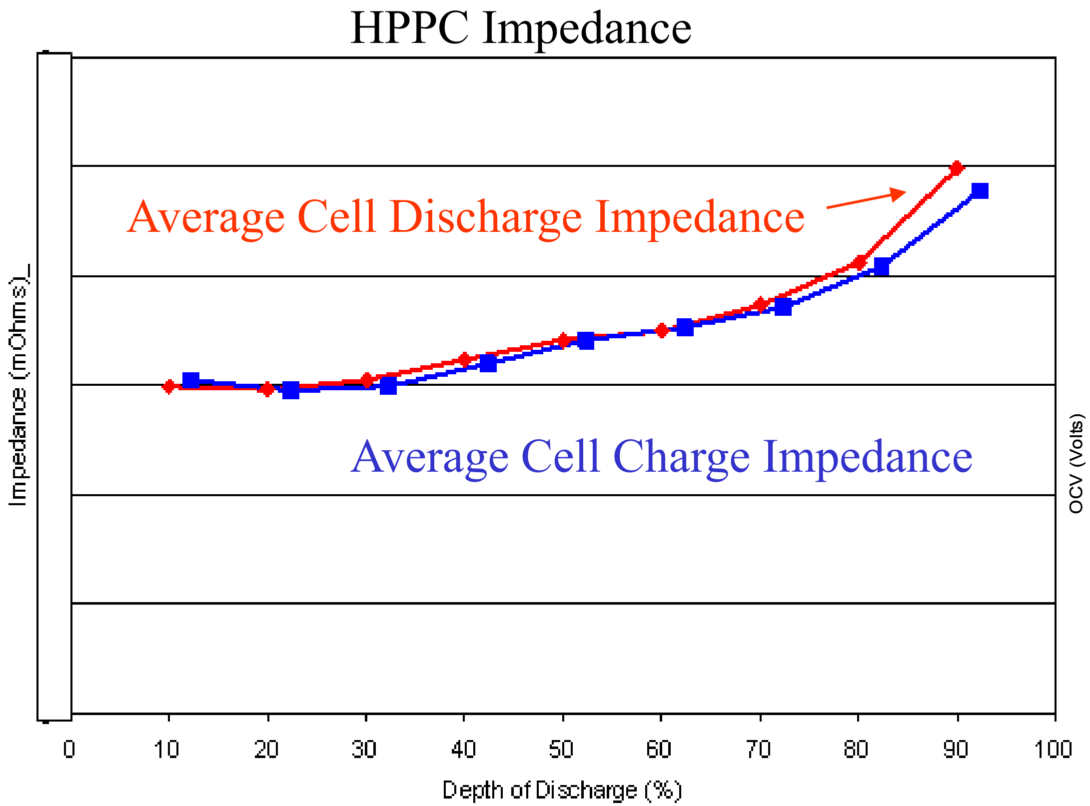


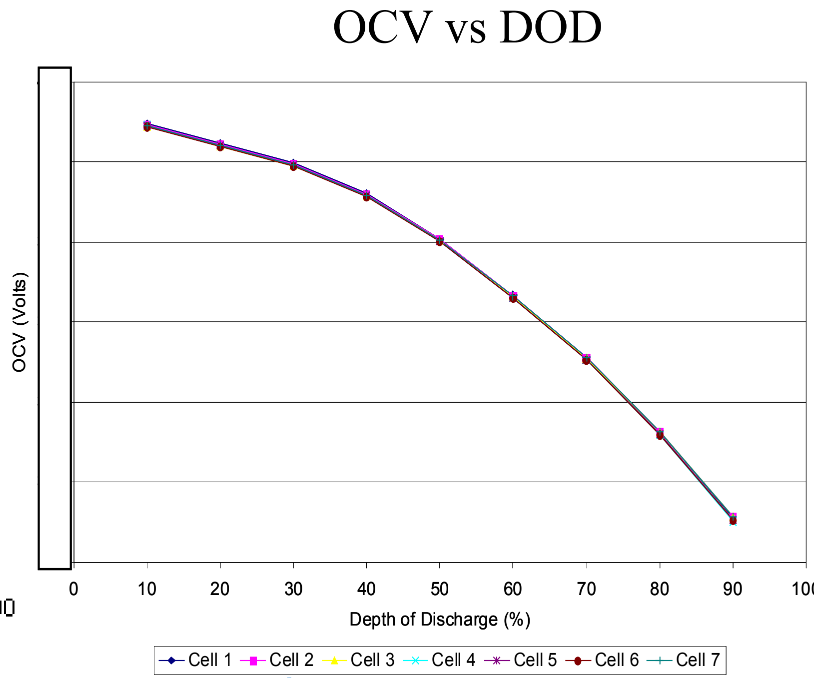


Electrical Evaluation: CPI HEV Module

- Electrical Study – HPPC and Voltage Performance under US06
- Consisting of eight (8) G4.3 LG Chem MnO_2 cells.



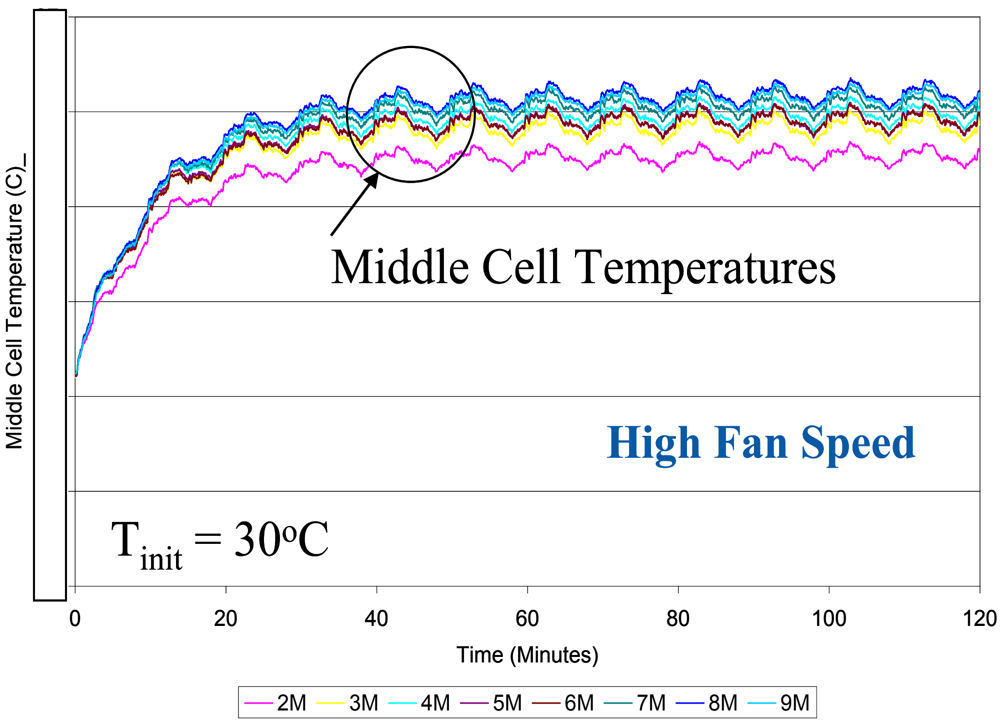


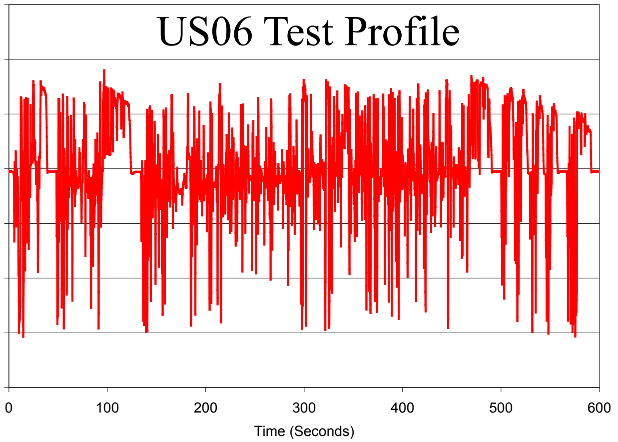


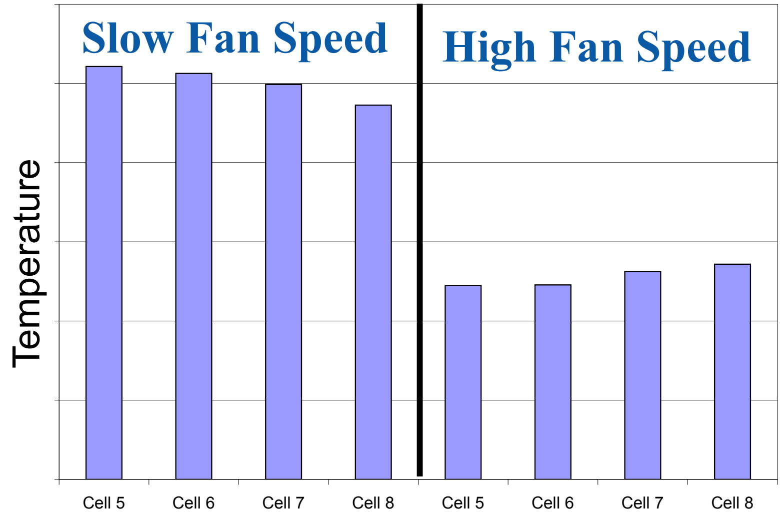
Thermal Evaluation: CPI HEV Module

- Tested simulating real conditions and operation
- Used different power profiles and ambient conditions
- Excellent thermal performance (2 C ΔT)

Continuous US06 Cycling

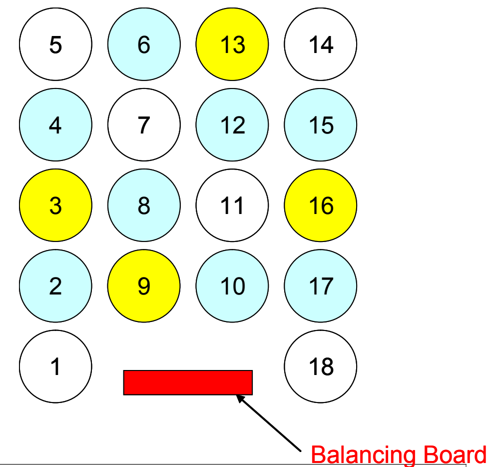






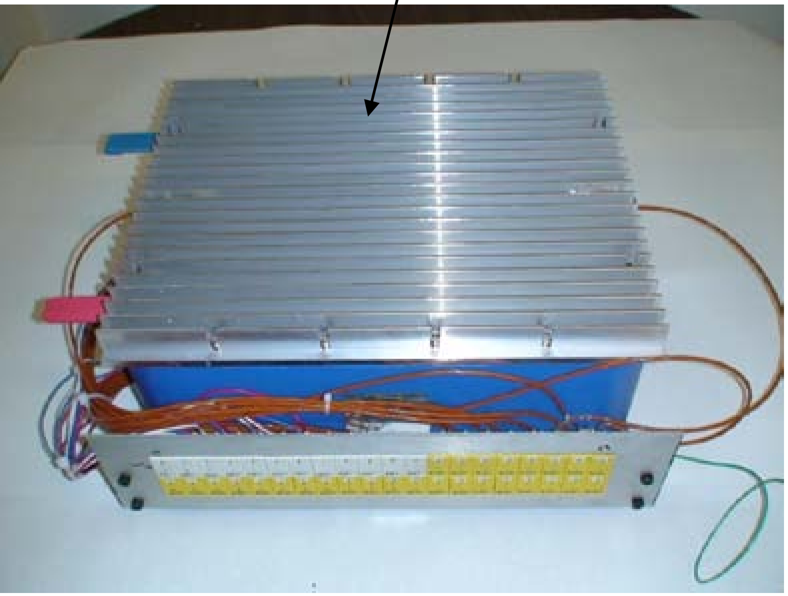
Thermal performance improved with higher air flow rate

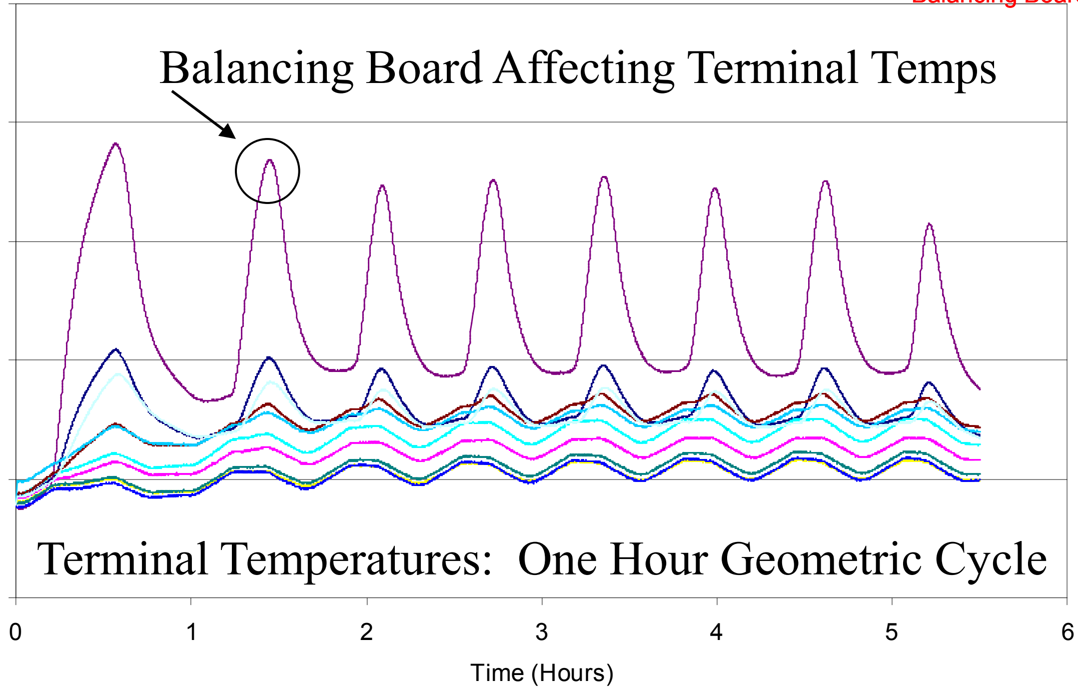
Thermal Evaluation: Nesscap Ultracap Module



- Tested as part of USABC deliverable
- Eighteen (18) symmetric carbon-carbon ultracapacitors
- Tested under realistic conditions and operation
- Used different power profiles and chamber temperatures

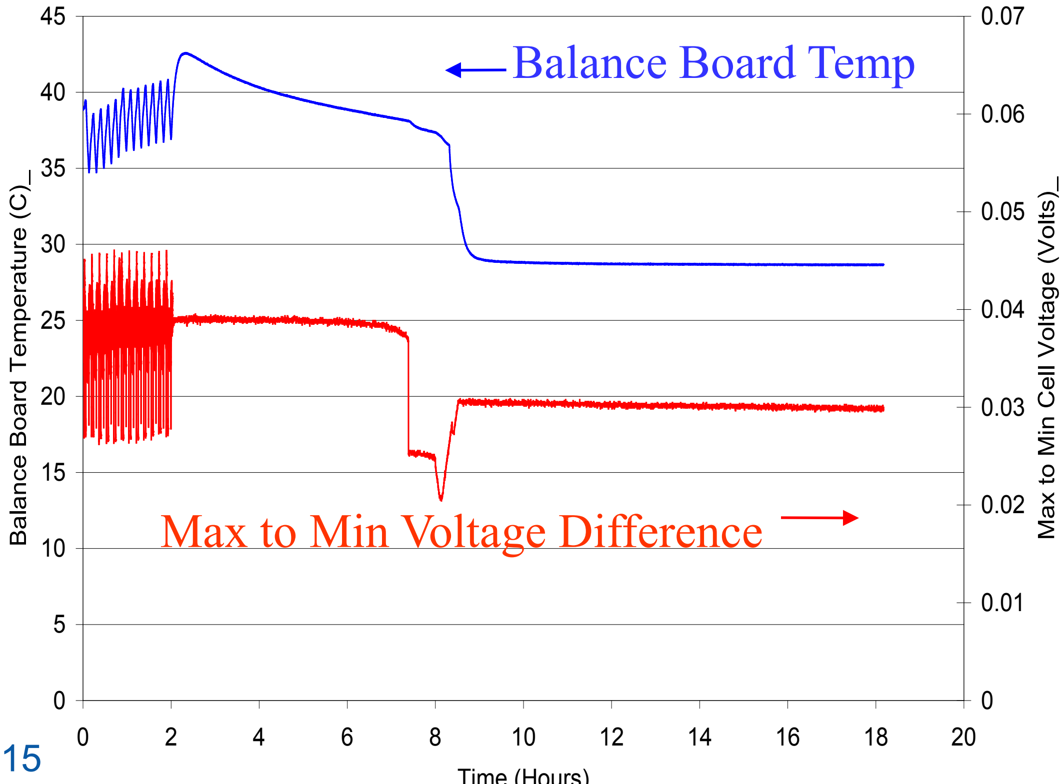
Heat from cells are conducted through the ends to the case and the rejected through the top metal heat sink/fins.

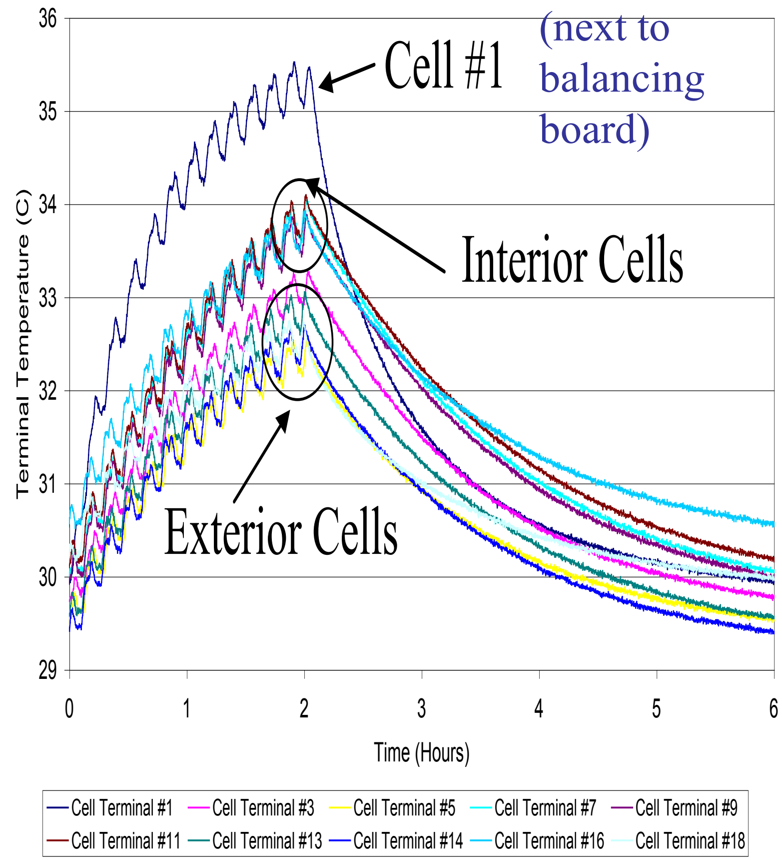




Thermal Evaluation: Nesscap Ultracap Module

- Continuous US06 cycling for two hours
- Balancing board did a good job equalizing cells
- Energy drain for balancing could be a concern





Temperature difference less than 1.5°C except for Cell #1 which heated due to balancing board.

Completed Fabrication of A New Calorimeter for Large, Liquid-Cooled HEV & PHEV Modules

- Used to measure heat generated from large batteries under real driving profiles and conditions
  - Liquid cooled capability
- The new calorimeter can test batteries 6 times larger than the existing NREL calorimeter
- Could be used for other automotive components such as power electronics & motors.

Completed System with Heating/Cooling Unit

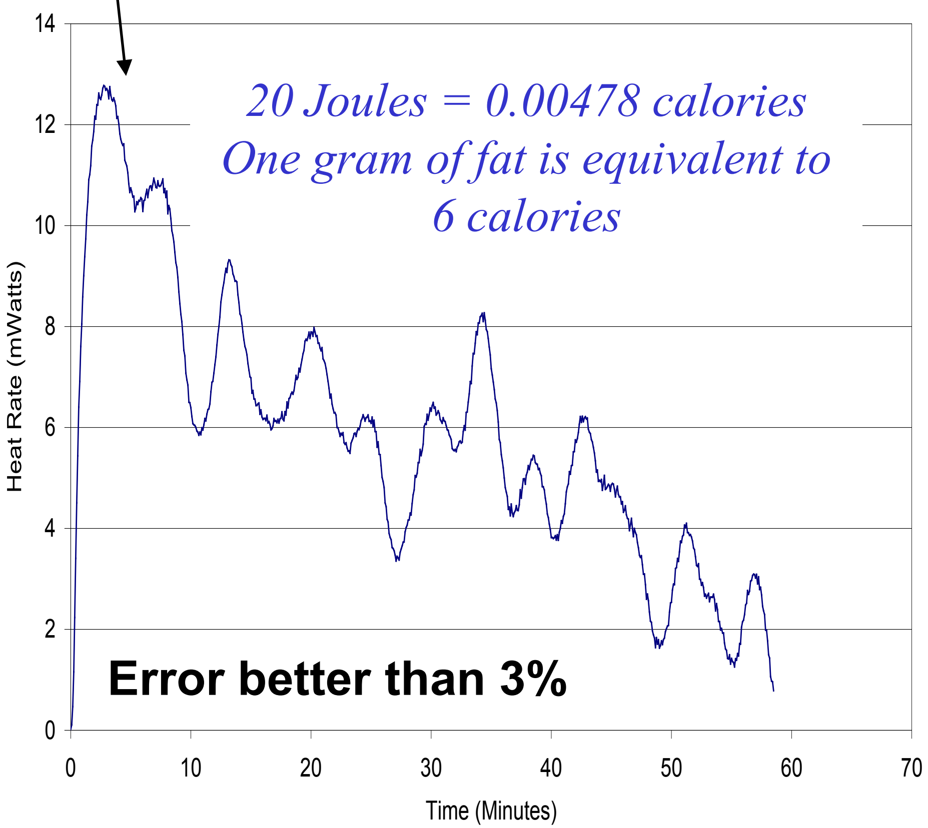
Flux Gauges of Test Chamber

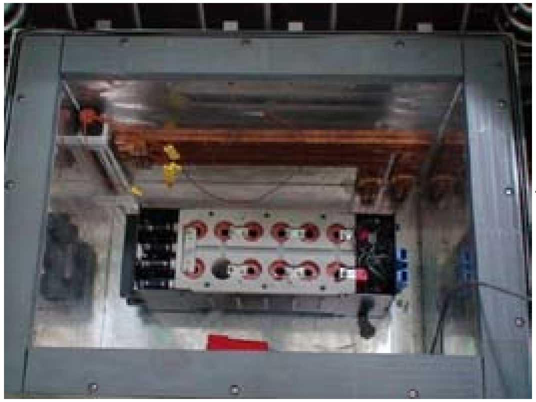
Test Chamber

Test Chamber in Isothermal Bath

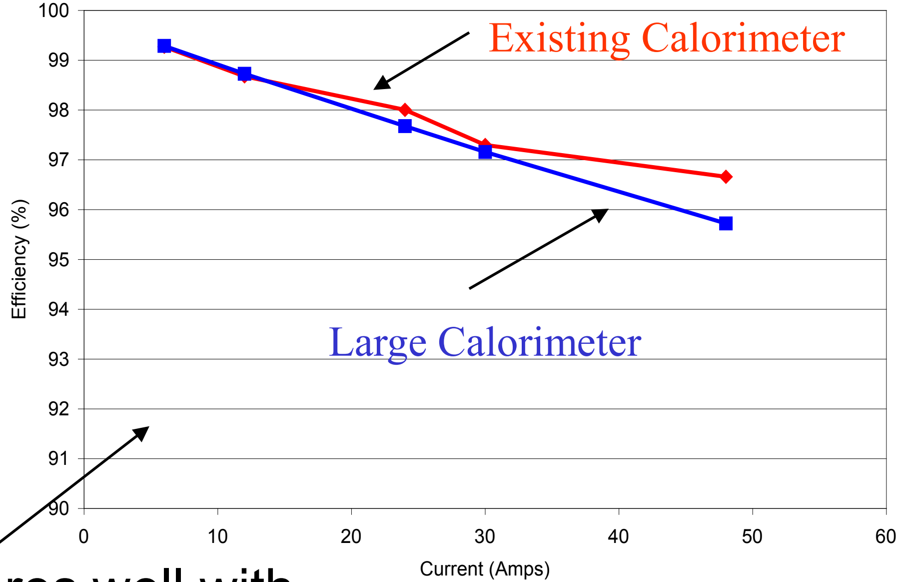
Large Calorimeter Calibration and Battery Testing

20.40 Joule electrical input released in a resistor
Measured response = 20.94 Joules



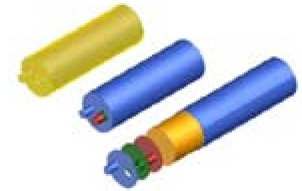


A large module in Test Chamber

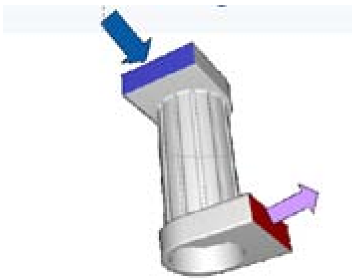


Large calorimeter's results compares well with the results of our existing calorimeter

Battery Thermal Modeling at NREL



Cell Characteristics



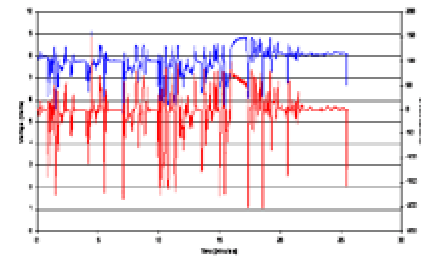
Module Cooling Strategy

Design Process

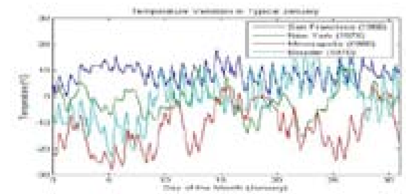
ANSYS | FLUENT | MATLAB

3D Component Analysis

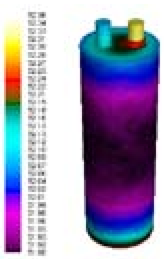
System Analysis

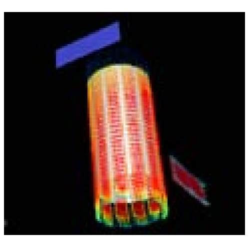


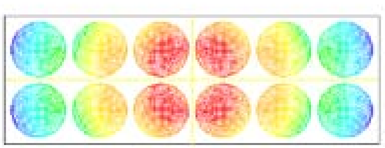
Operating Conditions

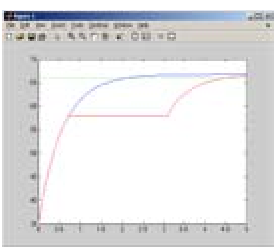


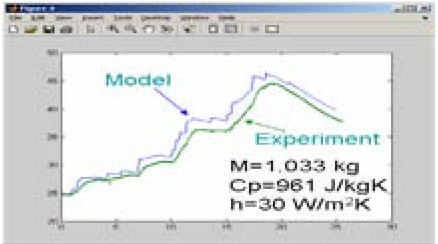
Battery Thermal Responses







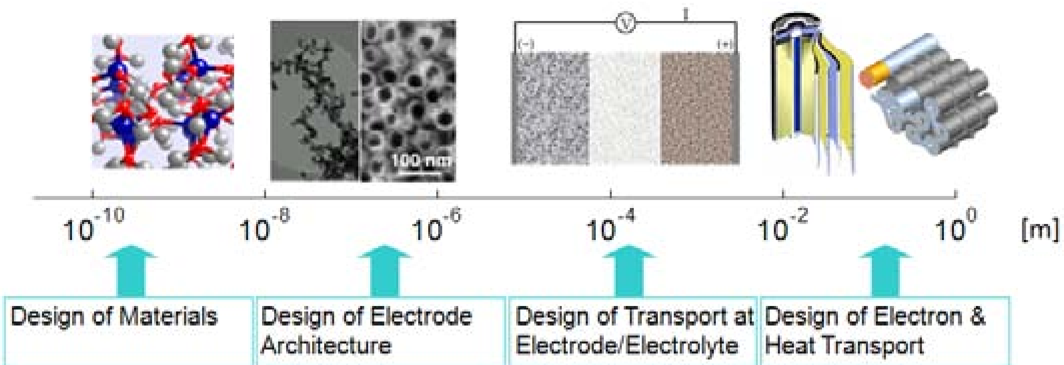




Multi-physics Battery Simulation Tool for Better Design and Management

Background

- Wide range of time and length scales physics
- Design improvements at different scales required
- Need to better understand the interaction among different scale physics



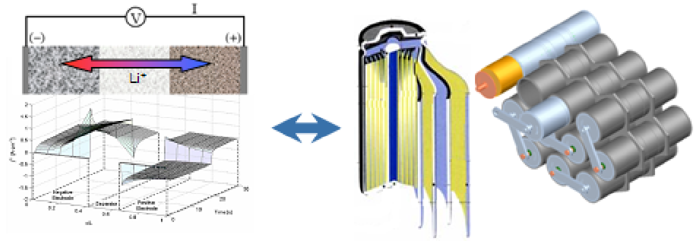
Objectives

- Develop computer-aided design tools for better cell design and management by working with industry
- Expand knowledge on the impacts of designs, usages, and managements on performance, life and safety of battery systems

Approach

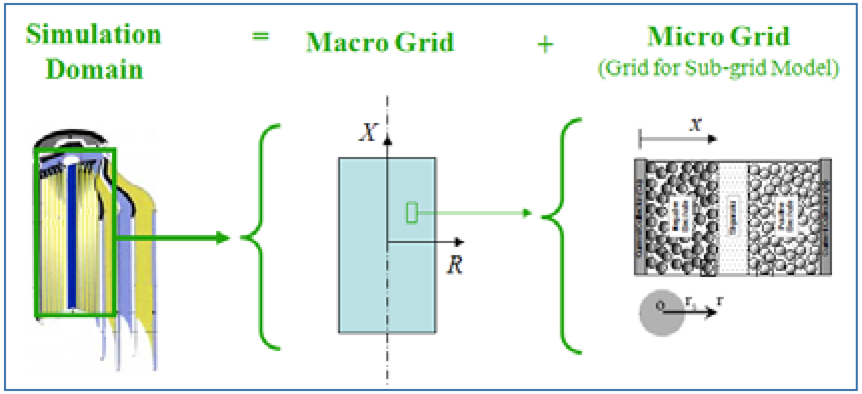
Multi-Scale Multi-Dimensional (MSMD) Model

- Capture macroscopic electron and heat transports, while maintaining model resolution to capture Li diffusion dynamics and charge transfer kinetics in electrode level scale
- Use separate domains for 1-D Newman-type electrochemical model and macro-scale heat and current transport model
- Physically couple the solution variables defined in each domain using multi-scale modeling schemes



Li Transport & Charge Transfer Kinetics

Electron Transport & Heat Transport

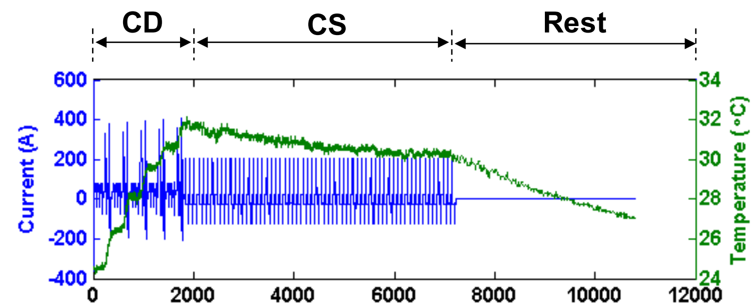


- Validate model for PHEV cell (electrical and thermal)
- Perform trade-studies for improved cell design and management

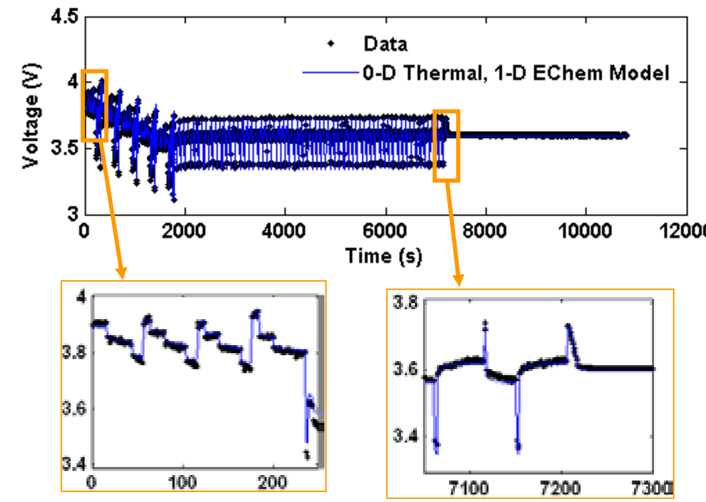
Model Validation

Thermal imaging test of three 41 Ah cells

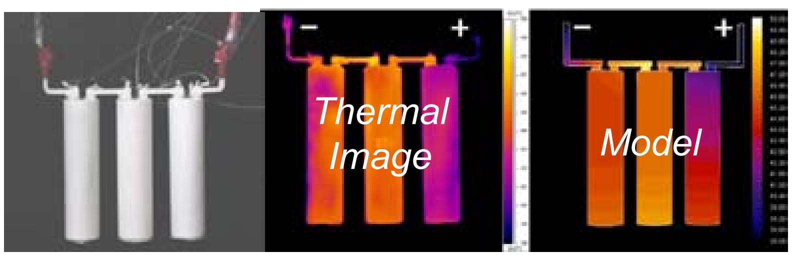
1) <u>Cycle</u>: USABC PHEV10 profile
(5xCD, 60xCS)



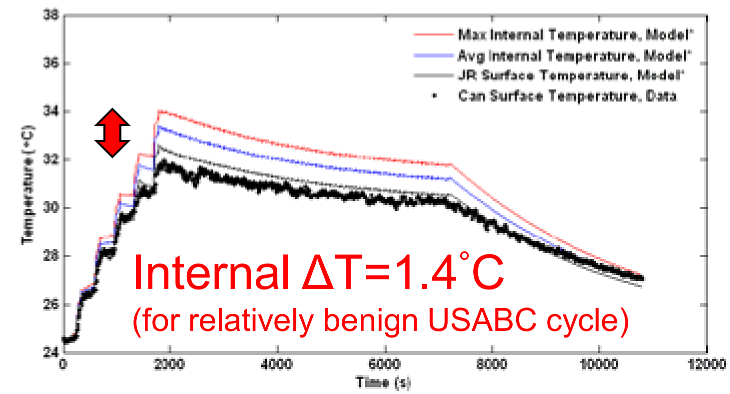
2) <u>1-D EChem model</u> well-matched to voltage data. Critical for correct heat generation prediction.



3) <u>Thermal-only model</u> used to quantify boundary conditions on center cell.

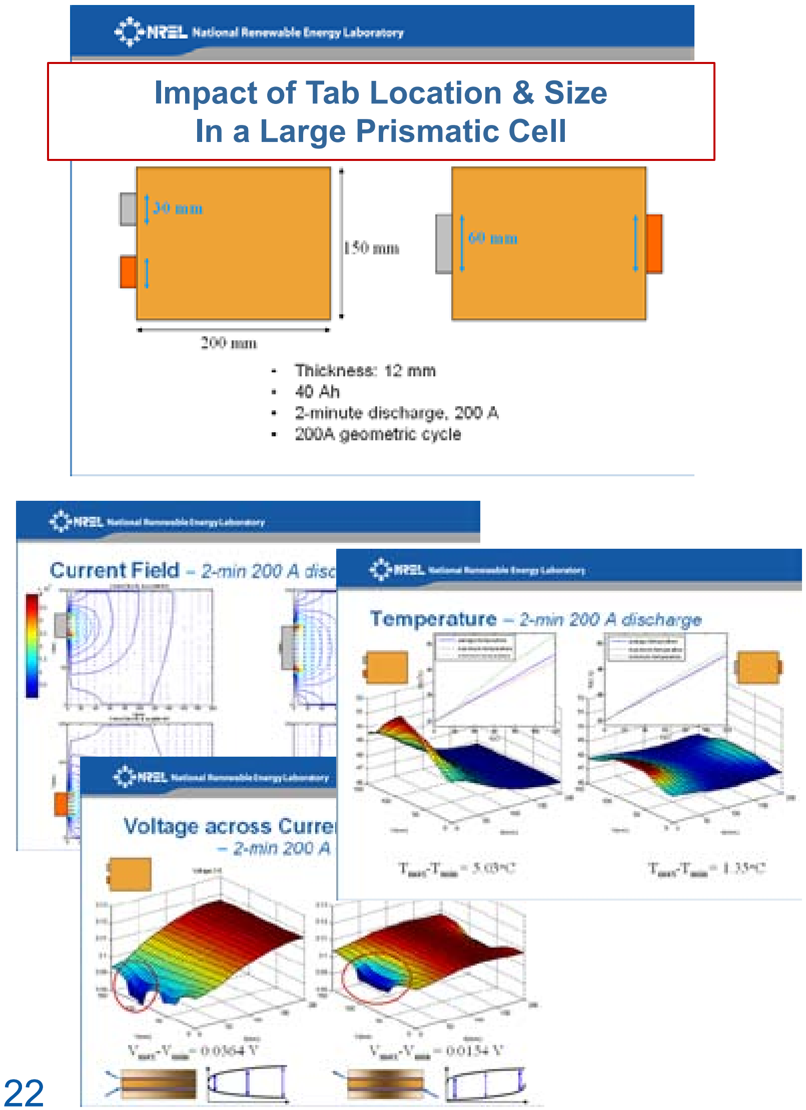


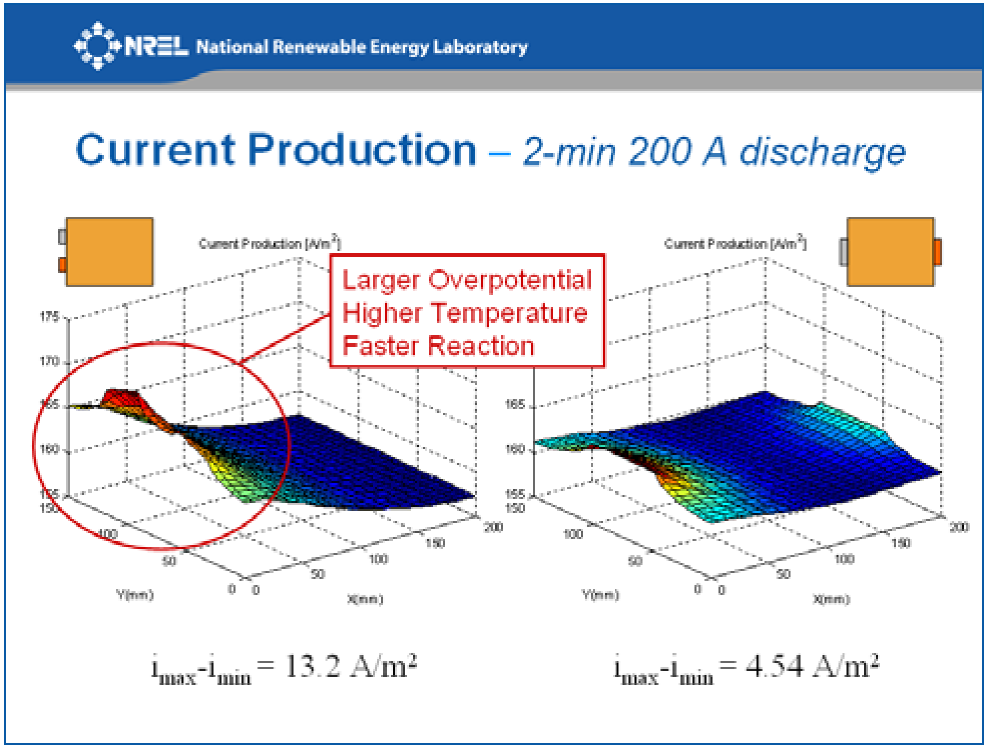
4) <u>3-D EChem/Thermal model</u> gives good prediction of cell skin temperature rise.



5) <u>Future</u>: Validate cell-internal temperatures.

AABC 08, Tampa, May 2008



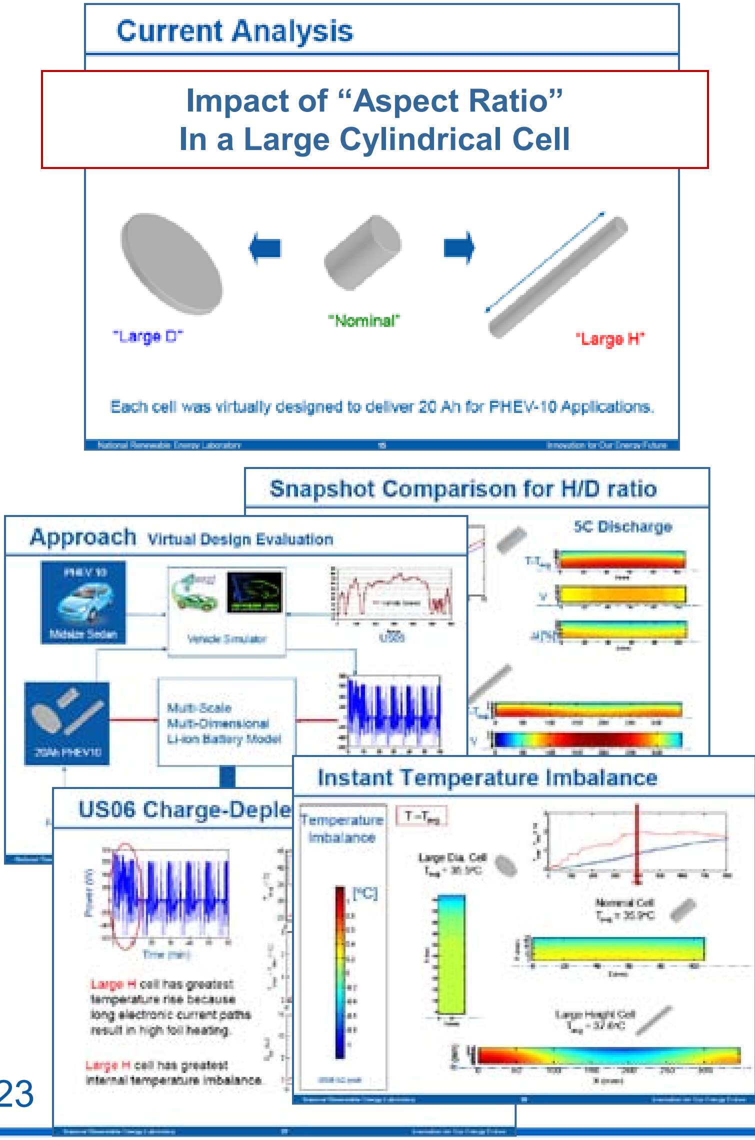


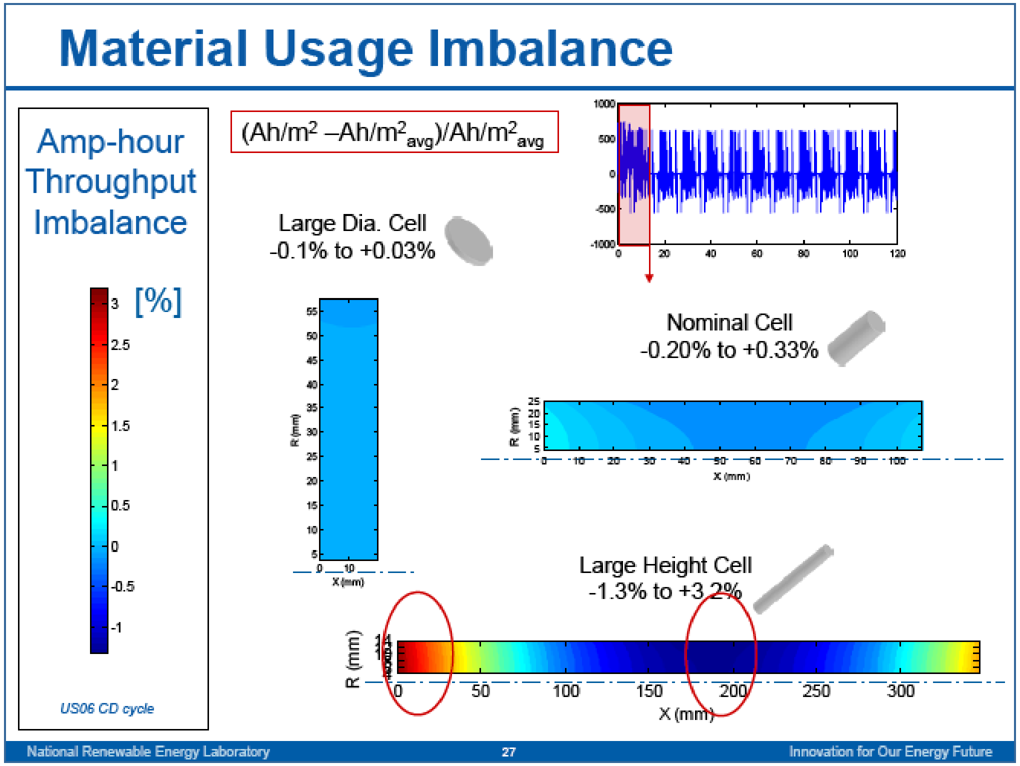
Accomplishments

- Micro-scale electrochemical processes and macroscopic heat and electron transports closely interact.
- Severe spatial non-uniformity can be caused by poorly designed macroscopic design features.

1. Thermal Characterization and Analysis Activity

214th ECS, Honolulu, Oct 2008





Accomplishments

Poorly designed electron and heat transport pathways can cause excessive nonuniform use of materials which lead to deterioration of performance and shorten the life of the battery.

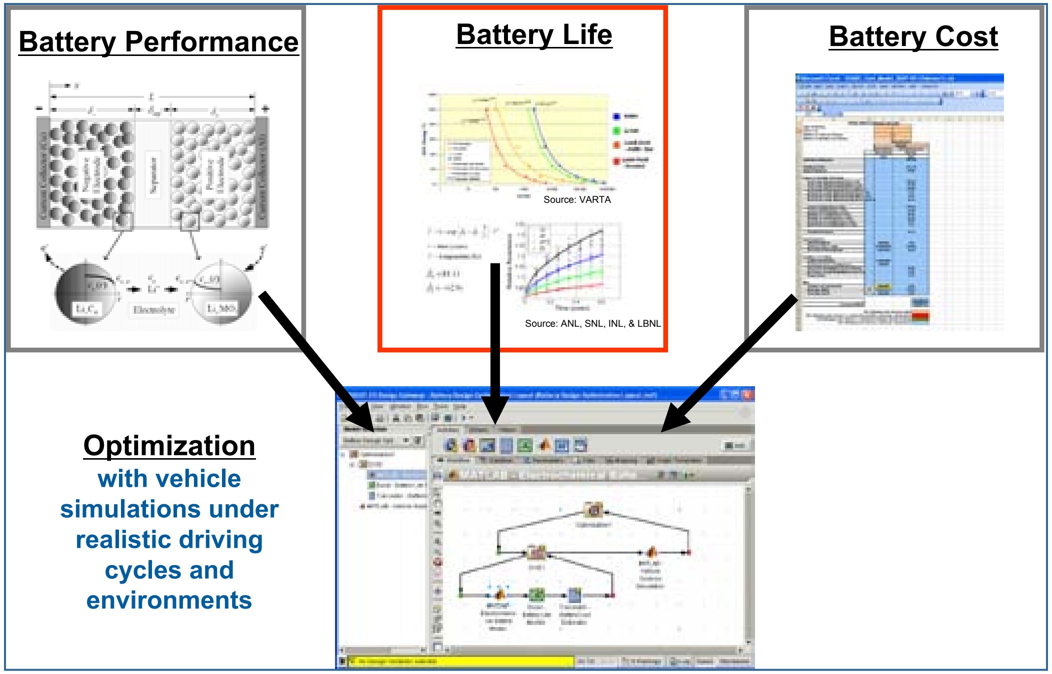
Future/Planned Work

- Continue working with HEV and PHEV battery developers on thermal characterization and analysis of batteries
  - EnerDel
  - A123 Systems
  - CPI/LG Chem
  - Johnson Controls - Saft
  - Others
- Use large calorimeter to measure heat from large PHEV modules and sub-packs
- Validate and refine the thermal-electrochemical model with experimental data and use it for developer's batteries
- Demonstrate the application of computer-aided battery design tool for PHEV prismatic cells
- Investigate cost effective approaches for thermal control of batteries when a PHEV is parked in hot environments

PHEV Battery Performance/Life/Cost Trade-off Analysis

Objectives

- Optimize energy storage system designs to:
  - minimize cost,
  - meet performance requirements,
  - meet life requirements
  - ensure reliability,
  - accelerate PHEV market penetration & fuel displacement.
- Evaluate real-world scenarios
  - climate, driving cycles, charging frequency.



- Life model represents greatest uncertainty (significant focus for FY09)
  - complex dependency on $t^{1/2}$, t, # cycles, T, V, ΔDOD.
- Life model requirements
  - use accelerated and real-time calendar and cycle life data as inputs,
  - is mathematically consistent with all empirical data,
  - is extendable to arbitrary usage scenarios (i.e., it is predictive).

Life Modeling Approach*

NCA dataset fit with empirical, yet physically justifiable formulas

Calendar fade
- SEI growth (partially suppressed by cycling)
- Loss of cyclable lithium
- $a_1(\Delta DOD, T, V)$

Cycling fade
- active material structure degradation and mechanical fracture
- $a_2(\Delta DOD, T, V)$

Resistance Growth

$$R = a_1 t^{1/2} + a_2 N$$

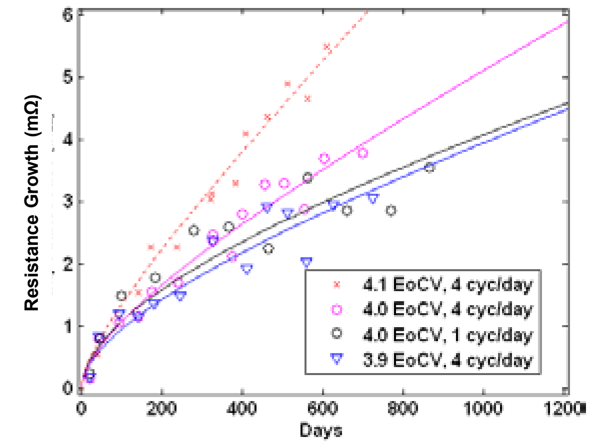
Relative Capacity

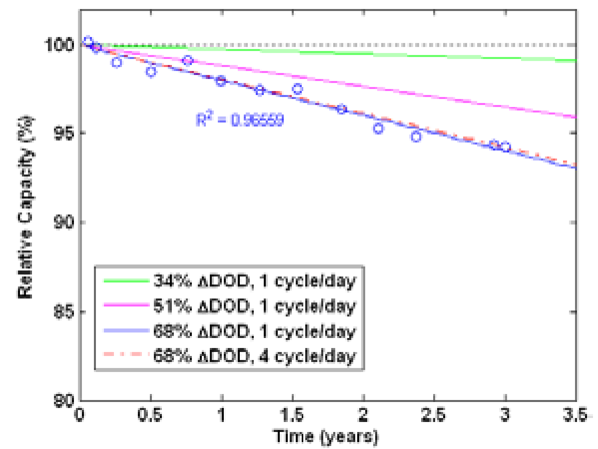
$$Q = \min(Q_{Li}, Q_{active})$$

$$Q_{Li} = d_0 + d_1 \times (a_1 t^{1/2})$$

$$Q_{active} = e_0 + e_1 \times (a_2 N)$$

Li-ion NCA chemistry





Data: John C. Hall, IECEC, 2006.

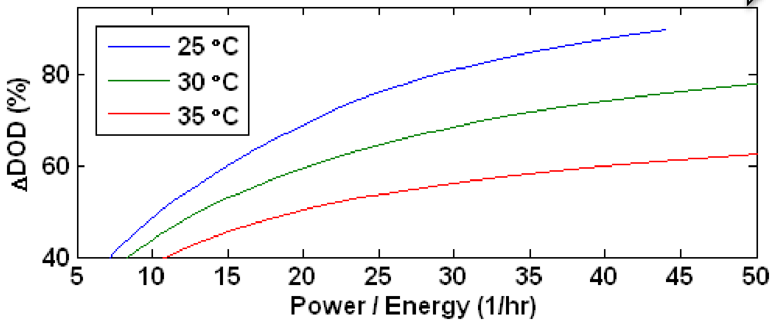
*K. Smith, T. Markel, A. Pesaran, "*PHEV Battery Trade-off Study and Standby Thermal Control*," 26th International Battery Seminar & Exhibit, Fort Lauderdale, FL, March, 2009.

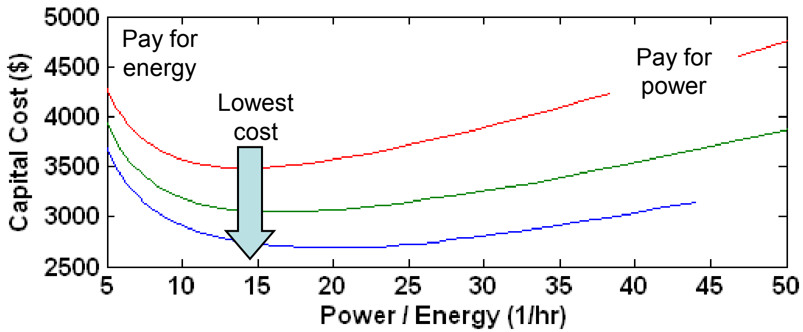
Example Trade-off Studies

Impact of requirements on battery size: Useable ΔDOD and cost

PHEV10: Assumed the battery has to last 10 years at various temperatures

Higher P/E increases useable ΔDOD



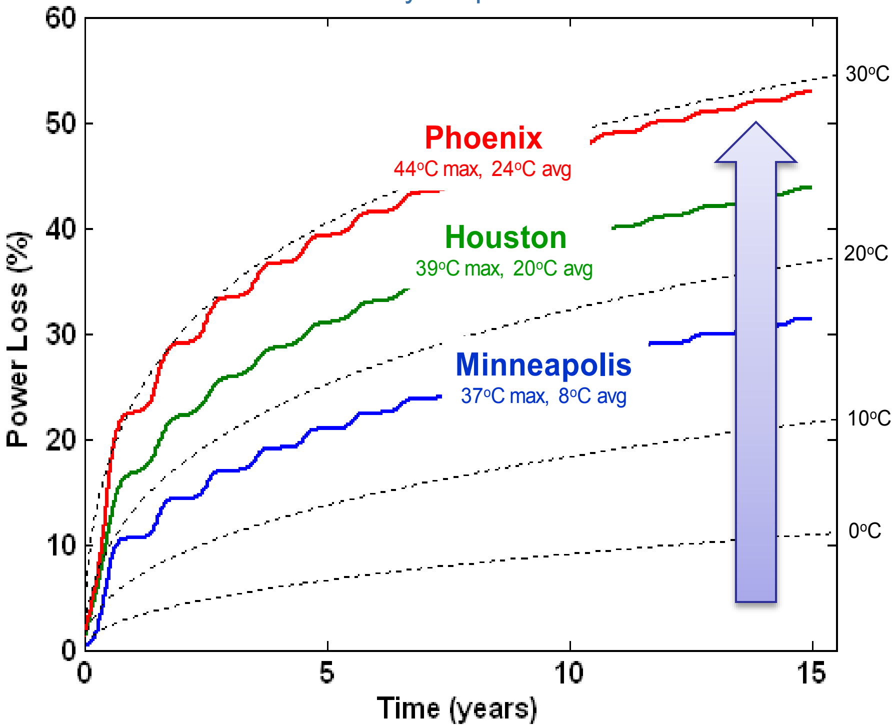


Reducing temperature exposure from 35°C to 25° reduces PHEV10 battery cost by $1000.

Impact of climate on power fade

Calendar fade model with Typical Meteorological Year (TMY) climate dataset

Assumed battery temperature = ambient



Some Li-ion technology must be sized with significant excess power to last 15 years.

2. Energy Storage Simulation and Analysis

Accomplishments

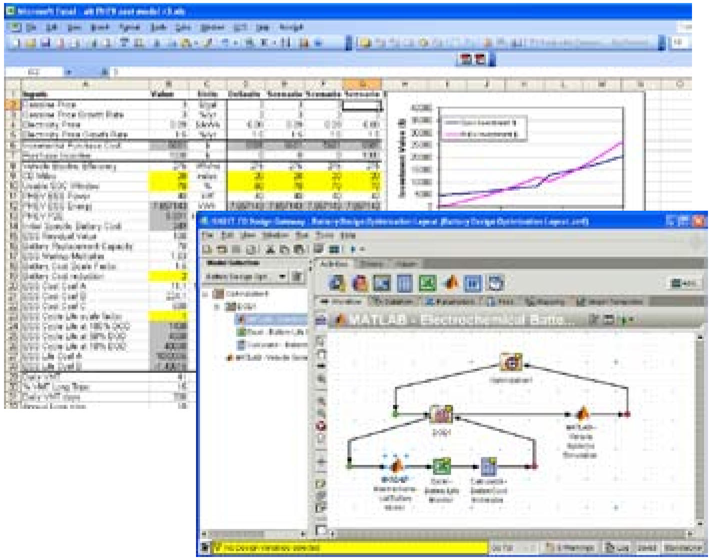
- Developed empirical life model for Li-ion carbon/NCA chemistry.
  (Additional comparison with DOE ANL/INL Gen II and NASA JPL datasets ongoing)
- Quantified impacts of life requirements (years and Temp.) on battery size and cost.
- Quantified calendar degradation for various climates in the USA.

Milestones

- Plug-In battery design - trade-off analysis (May 2009)
- Initial evaluation of EV battery swap concept (September 2009)

Future Work/Plans

- Extend models to understand
  - Implications of real world scenarios *(climate, driving profiles, charging frequency, …)*
  - Impact of various Li-ion chemistries.
- Work with others to obtain PHEV field data to validate the life model.
- Investigate the impact of ambient temperature and battery life on various EV infrastructure approaches such as
  - Fast charge
  - Battery swap



Applied Battery Research for Transportation

High Energy Battery Technology
Task 3: Abuse Tolerance Studies
Task 3.1: Abuse Behavior Modeling and Diagnostics

Multiple-Physics Safety Modeling
with Emphasis on Internal Short

- Safety is a major barrier for Li-ion batteries
- Need to develop safe and abuse-tolerant designs
- We are developing models in support of this

Modeling for Understanding Impacts of Battery Design Parameters on Thermal Runaway in Lithium-Ion Cells/Modules

3. Li-ion Thermal Abuse & Internal Short Modeling

FY09 Objective – *Model for Internal Short*

Develop and improve the "chemical reaction" model to evaluate recommended designs and/or materials that could enhance the safety tolerance of lithium-ion batteries, with emphasis on internal shorts

Research Focus – *Understanding Multi-physics of Internal Short*

- Understanding electrochemical response for short
- Understanding heat release for short event
- Understanding function and response of safety designs

Milestones

- Enhance 3-D Li-Ion battery abuse model (July 2009)
- Validate "electro-chemical-thermal" based battery abuse model (Sep 2009)

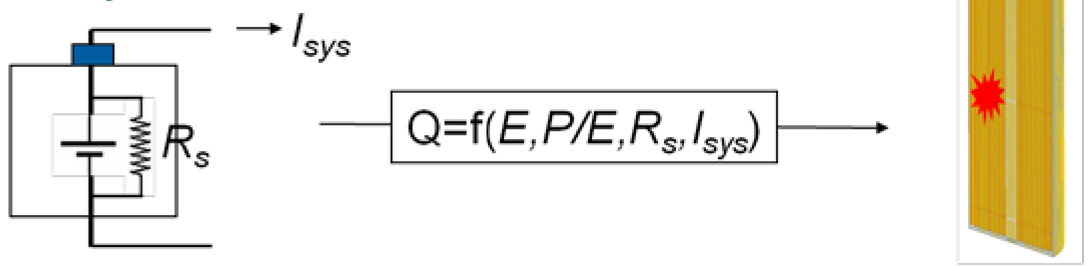
Approach – *Development & Validation of Multi-physics Model*

- Perform multiple physics modeling to expand understanding of internal shorts by linking the electrochemical cell model to the electro-thermal-abuse reaction kinetics model
- Collaborate with Sandia National Lab to plan and perform experimental tests for model validation

Accomplishment 1

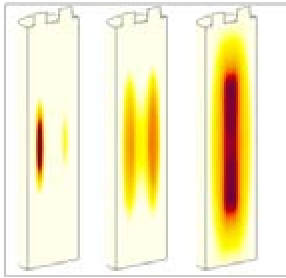
NREL's multi-physics model combination demonstrates that heating pattern at short events depends on various physical parameters such as nature of short, cell size, rate capability.

Example of Synergetic Model Combination for Study on Heat Release for Short



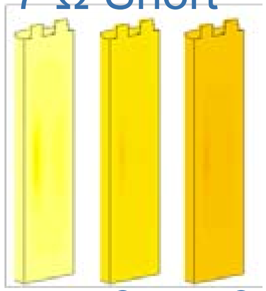
Electrical(Electrochemical) Short Cell Model — *3D Abuse Reaction Model*

30 mΩ Short



4s 8s 12s

7 Ω Short



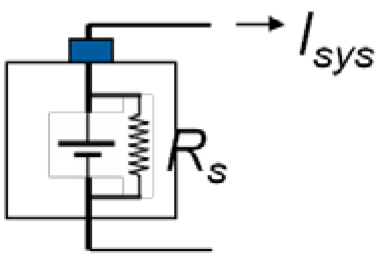
3m 6m 9m

- ✓ Schematic shows the concept of how we combine the electrochemical short cell model and 3D exothermic kinetics model.
- ✓ Contours show the difference in heating (temperature) for different electrical resistance shorts at the same cell.

Accomplishment 2

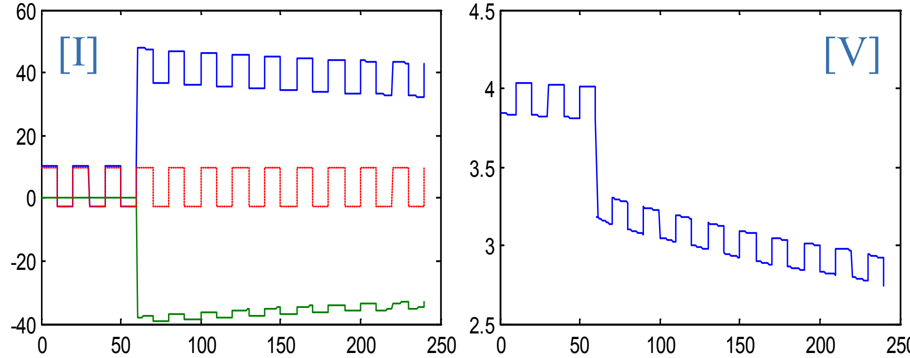
1D electrochemical short cell model results imply that detecting electric signal of internal shorts during battery operation is not easy for large format cells.

10sec 4C discharge 10sec 1C charge cycle,
R_s = 100 mΩ

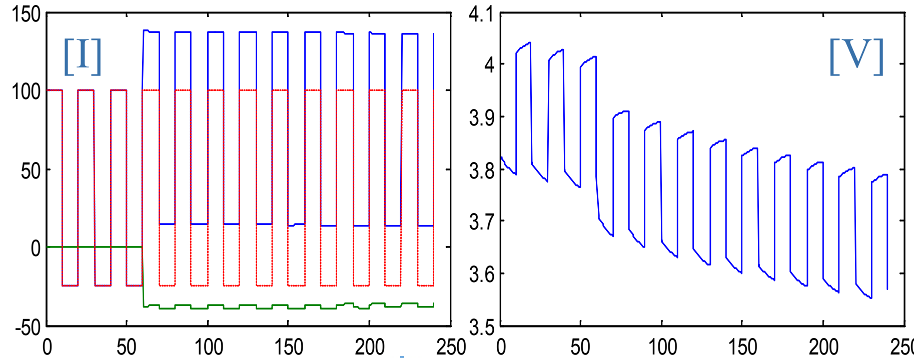


System current
Cell current
Short current

2.5 Ah cell



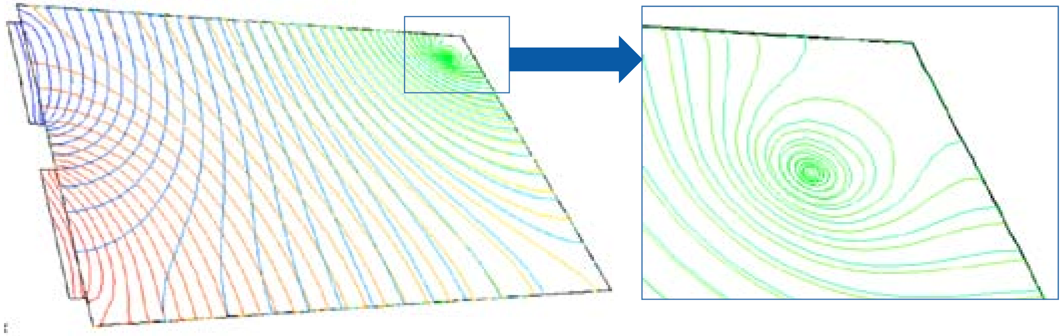
25 Ah cell



- ✓ Figures compare electrical responses (voltage and current) of short cells having different **capacities** under repeated discharge and charge cycle.

Accomplishment 3

Electrical, thermal and electrochemical natures significantly change for different type of internal shorts.



✓ Electric potential distribution under short between metal (Al, Cu) foils (e.g., metal debris penetration through electrode & separator layers)

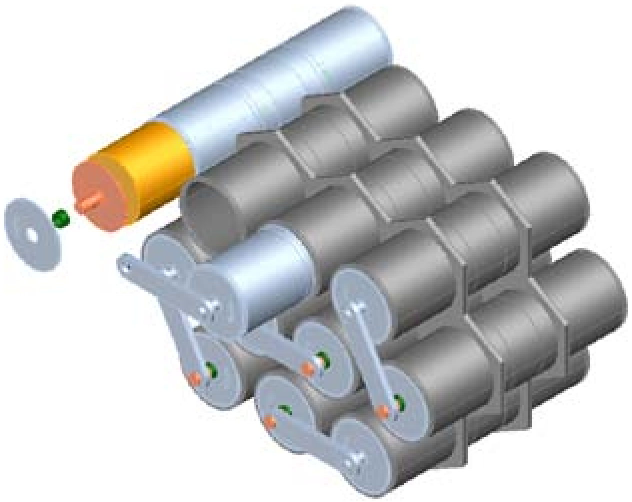
Planned Work

- Perform analysis for evaluating recommended safety designs such as functional separators (ceramic coated, shut-down feature) for various cell design parameters (materials, electrode thickness, cell capacity, etc)
- Design experimental apparatus for model validation through the collaboration with Sandia National Laboratory

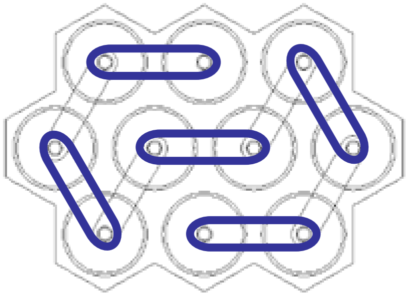
3D Thermal Propagation Model in a Module

- Developed a 3D cell and module geometry capturing impact of cell-to-cell interconnects on cell-to-cell thermal propagation.

CAD drawing of a 10-cell module



Grid for the 10-cell module

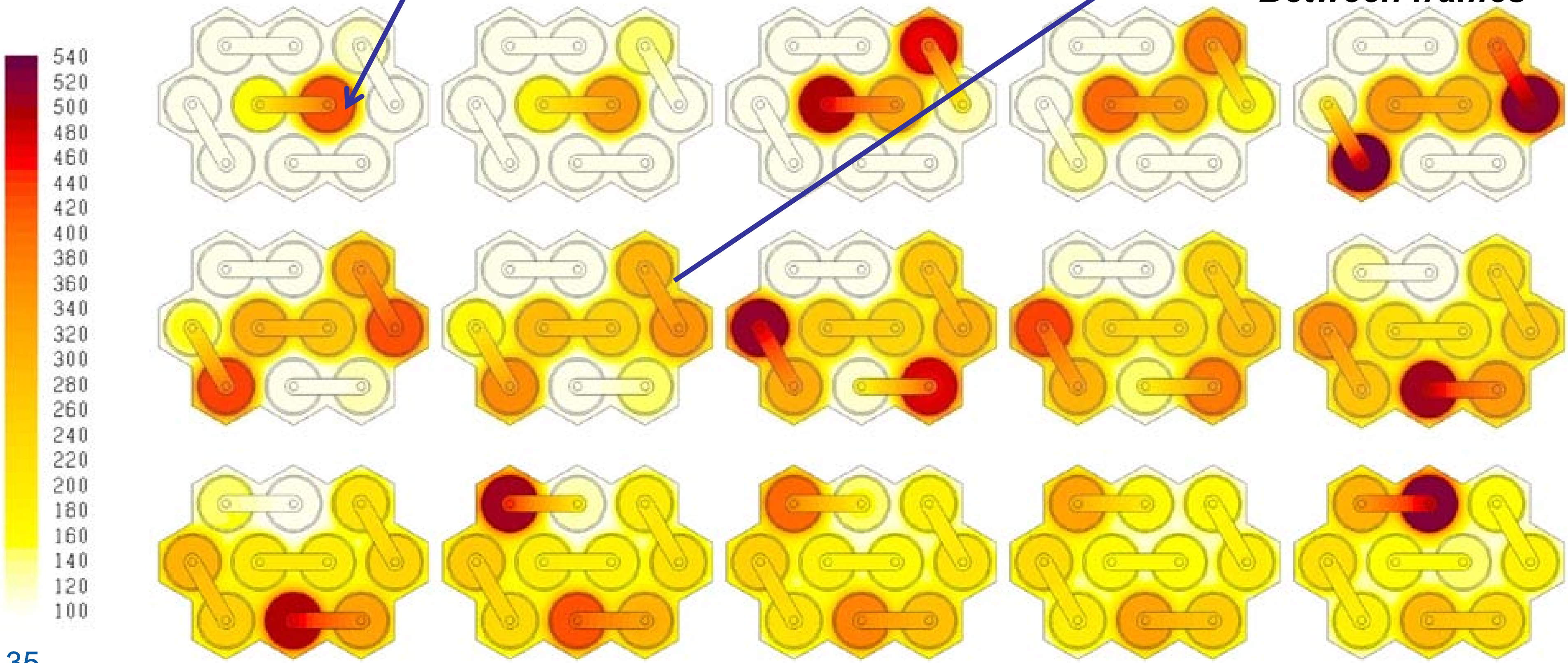


- 10 large cylindrical cells connected in series were inserted into a insulation holder
- Heat conduction through electrical connector dominates heat transfer between the cells in this module design

Thermal Propagation in a Module after Thermal Runaway of One Cell

Perspective View
Between frames

Top View 10 minutes apart between each frame/image



Overall Summary

- *NREL collaborates with industry and other national labs as part of the DOE integrated Energy Storage Program to develop advanced batteries for vehicle applications.*
- We moved toward achieving our goals, accomplish technical objectives, and delivered our milestones in the areas of
  1. Thermal characterization and analysis
  2. Energy storage simulation and analysis
  3. Li-ion thermal abuse reaction modeling
- Our activities support DOE goals, FreedomCAR targets, the USABC Tech Team, and battery developers.
- We developed tools and supported industry either through one-on-one collaborations or dissemination of information in international conferences and journals.

www.nrel.gov/vehiclesandfuels/energystorage/publications.html

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  - John Powell
  - Tony Markel
- Technical Guidance and Exchange with USABC and Energy Storage Tech Team
  - GM
  - Chrysler
  - Ford
  - Southern California Edison
- Input and Prototypes from Battery Developers
  - A123 Systems
  - Saft
  - Johnson Controls
  - CPI
  - LG Chem
  - JSR Micro
  - NessCap

Publications and Presentations

- G.H. Kim, K. Smith, "Three-Dimensional Lithium-Ion Battery Model," AABC-08 and the 4th International Symposium on Large Lithium-Ion Battery Technology and Application, May 13–16, 2008, Tampa, FL.
- G.H. Kim, K. Smith, "Multi-Scale Multi-Dimensional Model for Better Cell Design and Management," 1st International Conference on Li Batteries for Automotive Applications, September 15-17, 2008, Argonne, IL
- M. Keyser, J. Powell, K. Smith, G.H. Kim, A.A. Pesaran, "Thermal Evaluation of Advanced Batteries," Milestone Report, National Renewable Energy Laboratory, Golden, Colorado, August 2008
- T. Markel, K. Smith, A. A. Pesaran, "PHEV Energy Storage Performance/Life/Cost Trade-off Analysis," 8th Advanced Automotive Battery Conference, Tampa, FL, May 15, 2008.
- K. Smith, G.H. Kim, A. A. Pesaran, "Li-Ion Thermal Abuse Model-Methodology for Understanding Impacts of Battery Design Parameters on Thermal Runaway in Lithium-Ion Cells/Modules," The 77th Lithium Battery Technical/Safety Group Meeting, February 20-21, 2008, San Diego, CA
- G.H. Kim, A. A. Pesaran, K. Smith, "Thermal Abuse Modeling of Li-Ion Cells and Propagation in Modules," AABC-08 and the 4th International Symposium on Large Lithium-Ion Battery Technology and Application, May 13–16, 2008, Tampa, FL.
- A.A. Pesaran, G.H. Kim, K. Smith, "Thermal Abuse Modeling of Cylindrical and Prismatic Li-Ion Cells – Which Design Could Be More Abuse-Tolerant," 1st International Conference on Li Batteries for Automotive Applications, September 15-17, 2008, Argonne, IL

Publications and Presentations

- A.A. Pesaran, M. Keyser, Multiple presentations at FreedomCAR/USABC battery developers review meetings with battery-protected information, 2008-2009.
- K. Smith, T. Markel, and A.A. Pesaran, "Plug-In Hybrid Battery Trade-Off Analysis: Introduction," Milestone Report, National Renewable Energy Laboratory, Golden, CO, May 2008.
- G.-H. Kim, "Enhancement to Thermal Runaway Propagation Model for Lithium-Ion Cells and Battery Modules," Milestone Report, NREL, Golden, Colorado, July 2008.
- M. Keyser, et al. "FY 2008 Annual Energy Storage Program Report," Annual Report, NREL/TP-5400, National Renewable Energy Laboratory, Golden, CO, December 2008.
- G.H. Kim, K. Smith, "Multi-Scale Multi-Dimensional Li-Ion Battery Model for Better Design and Management," PRiME2008 and 214th ECS Meeting, Oct 12-17, 2008, Honolulu, HI
- A.A. Pesaran, "Battery Technology for Hybrid and Electric Vehicles - Opportunities and Challenges," Austin Energy AltCar Expo, October 17, 2008, Austin, TX
- K. Smith, G.H. Kim, E. Darcy, A. A. Pesaran, "Thermal/Electrical Modeling for Abuse Tolerant Design of Li-Ion Modules," NASA Aerospace Battery Workshop Huntsville, Alabama, November 18-20, 2008.
- A.A.. Pesaran, G.H. Kim, K. Smith, "Designing Safe Lithium Ion Battery Packs Using Thermal Abuse Models," Lithium Mobil Power 2008, December 8-9, 2008, Las Vegas, NV
- K. Smith, T. Markel, A. A. Pesaran, "PHEV Battery Trade-off Study and Standby Thermal Control," 26th International Battery Seminar & Exhibit, Fort Lauderdale, FL, March 17-19, 2009.